STIC Search Report
EIC 1700

USPTO

STIC Database Tracking Number: 101378

TO:	From:
Sin J Lee Location: CP3 9B05 Art Unit : 1752 September 4, 2003 Case Serial Number: 09/994808	John Calve Location: EIC 1700 CP3/4-3D62 Phone: 308-4139 John.Calve@uspto.gov

Search Notes

Sin,

No structures in req. file matched claim 3.

JoL

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Access DB# 101378

SEARCH REQUEST FORM

8

Scientific and Technical Information Center

Requester's Full Name: Sin J. Lee Examiner #: 76060 Date: 8-15-'03
Art Unit: 1752 Phone Number 30 5-0504 Serial Number: 09/994,808
Mail Box and Bldg/Room Location: 9B05 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Amine Compounds, Resist Compositions & Patterning Process

Inventors (please provide full names): Hatakeyama, Jun; Kobayashi, Tomohiro; Watanabe, Takeru; Nagata, Takeshi

Earliest Priority Filing Date: 11-28-01

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for the amine compound of claim #3.

( )

****

STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher:	NA Sequence (#)	STN
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#)	Questel/Orbit
Date Searcher Picked Up:	Bibliographic	Dr.Link
Date Completed:	Litigation	Lexis/Nexis
Searcher Prep & Review Time:	Fulltext	Sequence Systems
Clerical Prep Time:	Patent Family	WWW/Internet
Online Time:	Other	Other (specify)

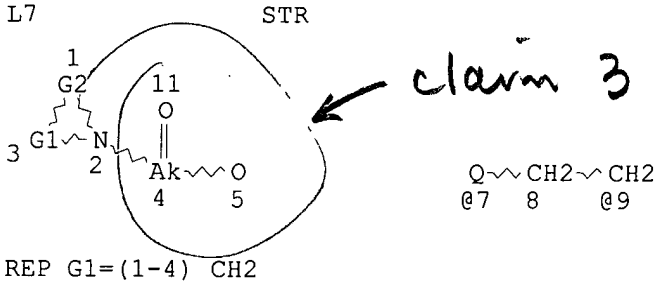
PTO-1590 (8-01)

Structure - claim 3

No hits.

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L2 SCR 1608 AND 1838 AND 1210 AND 1707
L3 SCR 1839 OR 2016 OR 2026 OR 1918 OR 1929 OR 2043 OR 1267 O
R 1700 OR 1304
L4 1038 SEA FILE=REGISTRY SSS FUL L1 AND L2 NOT L3
L7 STR



claim 3

REP G1=(1-4) CH2
REP G2=(0-5) 7-3 9-2
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
CONNECT IS E2 RC AT 5
DEFAULT MLEVEL IS ATOM
GGCAT IS SAT AT 4
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L9 0 SEA FILE=REGISTRY SUB=L4 SSS FUL L7

0 answers.

STIC Search Report
EIC 1700

USPTO

STIC Database Tracking Number: 101377

TO:	From:
Sin J Lee Location: CP3 9B05 Art Unit : 1752 September 4, 2003 Case Serial Number: 09/994808	John Calve Location: EIC 1700 CP3/4-3D62 Phone: 308-4139 John.Calve@uspto.gov

Search Notes

Structure - claim 2.

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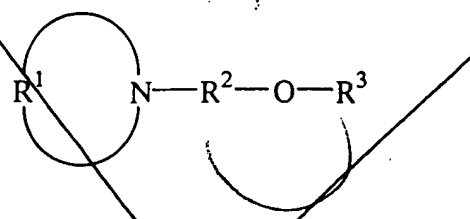
CLAIMS:

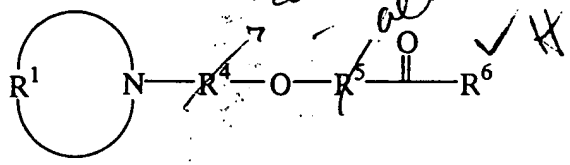
1. An amine compound of the following general formula (1):



(1)

wherein R^1 is a straight or branched alkylene group of 2 to 20 carbon atoms which may contain at least one carbonyl, ether, ester or sulfide group, R^2 is a straight or branched alkylene group of 1 to 10 carbon atoms, R^3 is a straight, branched or cyclic alkyl or alkoxy group of 1 to 20 carbon atoms which may contain a hydroxy group, ether group, carbonyl group, ester group, lactone ring or carbonate group, and R^2 and R^3, taken together, may form a ring with the oxygen atom.

2. An amine compound of the following general formula (2):



(2)

wherein R^1 is a straight or branched alkylene group of 2 to 20 carbon atoms which may contain at least one carbonyl, ether, ester or sulfide group, R^4 is a straight or branched alkylene group of 1 to 10 carbon atoms, R^5 is a single bond or a straight, branched or cyclic alkylene group of 1 to 20 carbon atoms, and R^6 is hydrogen or a straight, branched or cyclic alkyl or alkoxy group of 1 to 20 carbon atoms which may contain a hydroxy group, ether group, carbonyl group, ester group, lactone ring or carbonate group.

STIC Search Results Feedback Form

USPTO

EIC17000

Questions about the scope or the results of the search? Contact ***the EIC searcher or contact*:**

Kathleen Fuller, EIC 1700 Team Leader
308-4290, CP3/4-3D62

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art **not found**:*
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC/EIC1700 CP3/4 3D62

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```
=> file reg

FILE 'REGISTRY' ENTERED AT 14:43:27 ON 04 SEP 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES:    2 SEP 2003  HIGHEST RN 577952-45-5
DICTIONARY FILE UPDATES:   2 SEP 2003  HIGHEST RN 577952-45-5


=> d his

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L3             SCR 1839 OR 2016 OR 2026 OR 1918 OR 1929 OR 2043 OR 1267 OR 170
L4          1038 SEA FILE=REGISTRY SSS FUL L1 AND L2 NOT L3
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L6             3 S L5 SSS SAM  SUB=L4

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     FILE 'REGISTRY' ENTERED AT 14:13:12 ON 04 SEP 2003
L7            41 S L5 SSS FULL  SUB=L4
                SAVE L7 LEE808II/A

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L8            29 S L7

     FILE 'REGISTRY' ENTERED AT 14:14:30 ON 04 SEP 2003



=> d que stat L7
L1             STR
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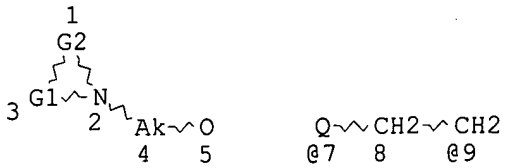
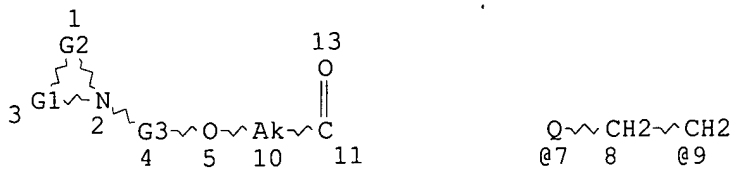


REP G1=(1-4) CH2
REP G2=(0-5) 7-3 9-2
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
CONNECT IS E2 RC AT 5
DEFAULT MLEVEL IS ATOM
GGCAT IS SAT AT 4
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L2 SCR 1608 AND 1838 AND 1210 AND 1707
L3 SCR 1839 OR 2016 OR 2026 OR 1918 OR 1929 OR 2043 OR 1267 OR 1700 OR 1304
L4 1038 SEA FILE=REGISTRY SSS FUL L1 AND L2 NOT L3
L5 STR



REP G1=(1-4) CH2
REP G2=(0-5) 7-3 9-2
REP G3=(1-15) C
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L7 41 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

100.0% PROCESSED 582 ITERATIONS 41 ANSWERS
SEARCH TIME: 00.00.01

=> file hca
FILE 'HCA' ENTERED AT 14:43:58 ON 04 SEP 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

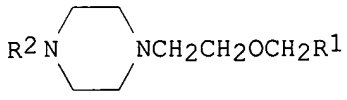
FILE COVERS 1907 - 28 Aug 2003 VOL 139 ISS 10
FILE LAST UPDATED: 28 Aug 2003 (20030828/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d L9 1-29 cbib abs hitind hitstr

L9 ANSWER 1 OF 29 HCA COPYRIGHT 2003 ACS on STN
127:331508 Novel substituted [2-(1-piperazinyl)ethoxy]acetic acid derivatives.
Duchene, Guy; Deleers, Michel; Bodson, Guy; Motte, Genevieve; Lurquin, Francoise (UCB S.A., Belg.; Duchene, Guy; Deleers, Michel; Bodson, Guy; Motte, Genevieve; Lurquin, Francoise). PCT Int. Appl. WO 9737982 A1 **19971016**, 44 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (French). CODEN: PIXXD2. APPLICATION: WO 1997-BE38 19970328. PRIORITY: BE 1996-310 19960410.

GI



I

AB Title compds. I [R1 = CONH2, CN, CO2H, CO2M, CO2R3; R2 = H, COR4, allyl, aralkyl; R3 = alkyl; R4 = alkoxy, haloalkoxy, aralkoxy, nitroaralkoxy, haloaralkoxy, haloalkyl; M = alkali metal] were prepd. as intermediates for I [R2 = diarylmethyl], which are in turn intermediates for the prepn. of I [R1 = CO2H, R2 = 4-ClC6H4CHPh, (4-FC6H4)2CH]. Thus, ClCH2CH2OCH2CONH2 was treated with piperazine to give I [R1 = CONH2, R2 = H] which was treated with (4-FC6H4)2CHCl to give I [R1 = CONH2, R2 = (4-FC6H4)2CH].

IC ICM C07D295-08
ICS C07D295-20

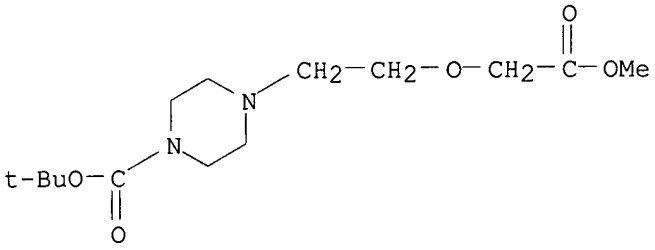
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 197968-56-2P 197968-65-3P 197968-72-2P 197968-77-7P 197968-78-8P
197968-80-2P 197968-82-4P 197968-84-6P 197968-91-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of piperazinylethoxyacetic acid derivs.)

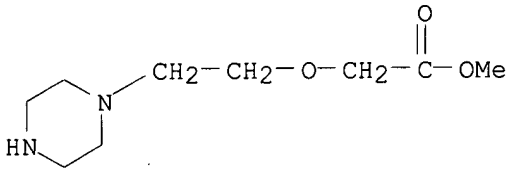
IT 83881-37-2P 83881-51-0P 150756-35-7P, Efletirizine 197968-59-5P
197968-61-9P 197968-63-1P 197968-70-0P 197968-74-4P
197968-86-8P 197968-87-9P 197968-89-1P 197968-93-7P 197968-98-2P
197969-01-0P 197969-03-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of piperazinylethoxyacetic acid derivs.)

IT **197968-80-2P**

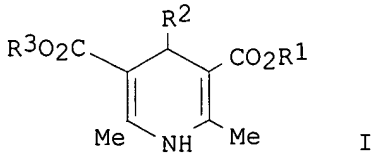
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of piperazinylethoxyacetic acid derivs.)
RN 197968-80-2 HCA
CN 1-Piperazinecarboxylic acid, 4-[2-(2-methoxy-2-oxoethoxy)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT **197968-61-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of piperazinylethoxyacetic acid derivs.)
RN 197968-61-9 HCA
CN Acetic acid, [2-(1-piperazinyl)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 2 OF 29 HCA COPYRIGHT 2003 ACS on STN
127:176348 Preparation of dihydropyridine derivatives as antagonists against tolerance to anticancer drugs or potentiators for anticancer drugs. Kiue, Akira; Miura, Teruhisa; Tasaka, Shigeyuki (Nikken Chemicals Co., Ltd., Japan; Kiue, Akira; Miura, Teruhisa; Tasaka, Shigeyuki). PCT Int. Appl. WO 9728125 A1 **19970807**, 46 pp. DESIGNATED STATES: W: CA, US; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1997-JP84 19970117. PRIORITY: JP 1996-33088 19960129; JP 1996-263799 19960913.
GI



I

AB The title compds. (I; R1 = disubstituted aminoalkyl, piperazinylalkyl, thiazolylalkyl, etc.; R2 = C3-10 alkyl, alkenyl, alkynyl, etc.; R3 = lower alkyl, pyridylmethyl, pyridylethyl, etc.) are prepd. I are useful as antagonists against tolerance to anticancer drugs or potentiators for anticancer drugs. Thus,3-pyridylmethyl acetoacetate was refluxed with

2-(N-benzyl-N-methylamino)ethyl 3-aminocrotonate and n-valeraldehyde in iso-PrOH for 6 h to give 52% I (R1 = 3-pyridylmethyl, R2 = Bu, R3 = CH2CH2NMeCH2C6H5), which showed IC50 of 465 X 10-7 M against high potassium induced contraction when tested with rat.

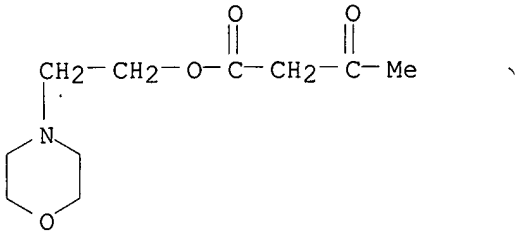
IC ICM C07D211-90
ICS C07D401-12; C07D401-14; C07D417-12; C07D417-14; A61K031-455; A61K031-495; A61K031-535

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

IT 66-25-1, Caproic aldehyde 110-62-3, n-Valeraldehyde 123-15-9 123-72-8, Butanal 124-19-6, Nonanal 6131-49-3 14205-39-1, Methyl 3-aminocrotonate 22502-03-0, 2-Methoxyethyl acetoacetate 50899-05-3, 3-Pyridylmethyl acetoacetate 50899-06-4, 2-Pyridylmethyl acetoacetate **50899-08-6**, Morpholinoethyl acetoacetate **55985-43-8** 56019-57-9, 2-(2-Pyridyl)ethyl acetoacetate 62595-86-2 71784-33-3 116395-62-1 128995-75-5, 4-Pyridylmethyl acetoacetate 137338-19-3 **177649-72-8** 193822-38-7 **193822-39-8** 193822-40-1 193822-41-2 193822-42-3 193822-43-4 193822-44-5 193822-45-6 193822-46-7 193822-47-8 193822-48-9 193822-49-0 193822-50-3 193822-53-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of dihydropyridine derivs. as antagonists against tolerance to anticancer drugs or potentiators for anticancer drugs)

IT **50899-08-6**, Morpholinoethyl acetoacetate **55985-43-8** **177649-72-8** **193822-39-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of dihydropyridine derivs. as antagonists against tolerance to anticancer drugs or potentiators for anticancer drugs)

RN 50899-08-6 HCA
CN Butanoic acid, 3-oxo-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)



RN 55985-43-8 HCA
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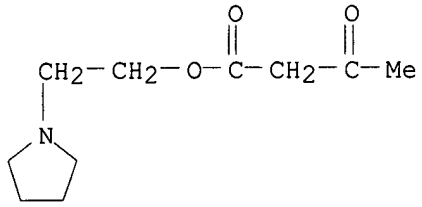
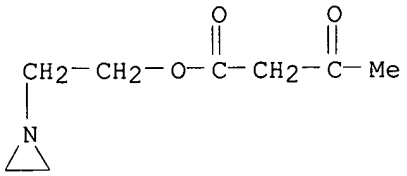
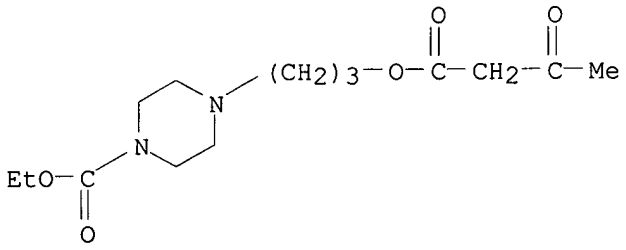


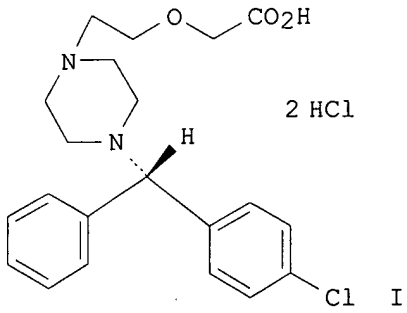
RN 177649-72-8 HCA
CN Butanoic acid, 3-oxo-, 2-(1-aziridinyl)ethyl ester (9CI) (CA INDEX NAME)



RN 193822-39-8 HCA
CN 1-Piperazinecarboxylic acid, 4-[3-(1,3-dioxobutoxy)propyl]-, ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 3 OF 29 HCA COPYRIGHT 2003 ACS on STN
125:221786 Catalytic enantioselective synthesis of the second generation histamine antagonist cetirizine hydrochloride. Corey, E. J.; Helal, Christopher J. (Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA). Tetrahedron Letters, 37(28), 4837-4840 (English) **1996**. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 125:221786. Publisher: Elsevier.
GI



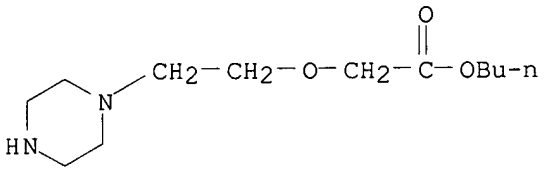
AB The first enantioselective synthesis of cetirizine hydrochloride (I) has been developed using the highly stereospecific chiral oxaborolidine (CBS) redn. of 4-[.eta.6-chromium tricarbonylbenzoyl]chlorobenzene to establish the benzhydryl stereocenter. The chromium tricarbonyl unit also served as the stereocontroller to allow the stereospecific displacement of hydroxyl by amino at the benzylic stereocenter.
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 29
IT 14869-41-1P 68448-72-6P 69811-90-1P 174004-10-5P

181119-50-6P 181119-55-1P 181119-59-5P 181119-68-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective synthesis of cetirizine dihydrochloride via chiral oxaborolidine redn. of (chromium tricarbonylbenzoyl)chlorobenzene)

IT **181119-50-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective synthesis of cetirizine dihydrochloride via chiral oxaborolidine redn. of (chromium tricarbonylbenzoyl)chlorobenzene)

RN 181119-50-6 HCA

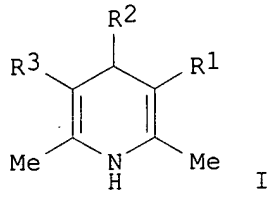
CN Acetic acid, [2-(1-piperazinyl)ethoxy]-, butyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 4 OF 29 HCA COPYRIGHT 2003 ACS on STN

125:33664 Preparation and formulation of dihydropyridines as PAF antagonists and antineoplastic potentiators. Tasaka, Shigeyuki; Miura, Teruhisa; Kiue, Akira; Seki, Taketsugu; Sano, Tetsuro; Kamakura, Mie; Fujita, Masakazu (Nikken Chemicals Co., Ltd., Japan). PCT Int. Appl. WO 9604268 A1 **19960215**, 48 pp. DESIGNATED STATES: W: CA, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1995-JP1507 19950728. PRIORITY: JP 1994-196204 19940729; JP 1995-79331 19950313.

GI



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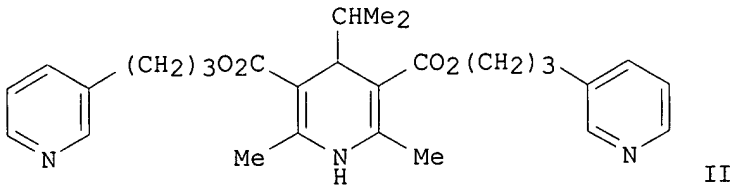


II

AB The title compds. I [R1 represents CO2A(3-pyridyl), and A represents C3-C6 linear alkylene which may have an intervening piperazine ring; R2 represents C2-C10 alkyl, alkenyl or alkynyl, substituted lower alkyl or alkenyl, or optionally substituted cycloalkyl; R3 represents the same group as R1 or CO2R4, and R4 represents optionally substituted lower

alkyl], useful as PAF antagonists, antineoplastic potentiators, and thromboxane A2 inhibitors, are prepd. The title compd. II (prepn. given) in vitro at 10-5 mol gave 82.7% inhibition of PAF-induced platelet aggregation. II in vitro showed IC50 of > 300 x 10-7 M against KCl-induced contraction of rat artery, vs. IC50 of 0.8 x 10-7 M for nimodipine, and IC50 of 23.5 x 10-7 M for verapamil.

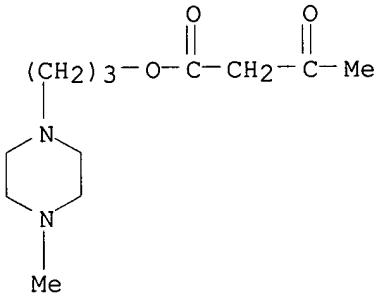
IC ICM C07D401-12
ICS C07D401-14; A61K031-445; A61K031-495

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

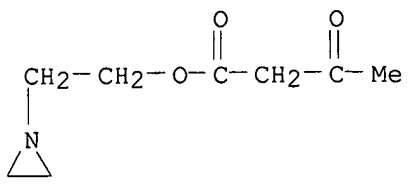
IT 66-25-1, Capronaldehyde 78-84-2 93-53-8, 2-Phenylpropionaldehyde 96-17-3 97-96-1 104-53-0, Benzenepropanal 106-23-0, Citronellal 107-86-8, 3-Methyl-2-butenal 122-78-1, Phenylacetaldehyde 123-05-7, 2-Ethylhexylaldehyde 123-15-9, 2-Methylvaleraldehyde 123-72-8, Butyl aldehyde 124-19-6, Nonylaldehyde 591-60-6, Butyl acetoacetate 623-30-3, 3-(2-Furyl)acrolein 947-91-1, Diphenylacetaldehyde 1846-68-0, 2-Octynal 2043-61-0, Cyclohexanecarboxaldehyde 2987-16-8 5435-64-3, 3,5,5-Trimethylhexanal 7664-41-7, Ammonia, reactions 14205-39-1 **50899-09-7** 54527-73-0 61382-53-4 65193-87-5, 2-Cyanoethyl acetoacetate 86575-68-0 100303-72-8 103839-99-2, 3-(3-Pyridyl)propyl acetoacetate 128995-75-5, 4-Pyridylmethyl acetoacetate 176906-73-3 176906-75-5, 3-(4-Pyridyl)propyl acetoacetate 176906-76-6, 3-(2-Pyridyl)propyl acetoacetate 176906-77-7 176906-79-9, 4-(3-Pyridylbutyl) acetoacetate 177030-31-8, 2-(3-Pyridyloxy)ethyl acetoacetate 177649-32-0 177649-71-7 **177649-72-8** 177649-73-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of dihydropyridines as PAF antagonists and antineoplastic potentiators)

IT **50899-09-7 177649-72-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of dihydropyridines as PAF antagonists and antineoplastic potentiators)

RN 50899-09-7 HCA
CN Butanoic acid, 3-oxo-, 3-(4-methyl-1-piperazinyl)propyl ester (9CI) (CA INDEX NAME)



RN 177649-72-8 HCA
CN Butanoic acid, 3-oxo-, 2-(1-aziridinyl)ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 5 OF 29 HCA COPYRIGHT 2003 ACS on STN
124:261768 Urea-containing hydroxyethylamine peptides as retroviral protease inhibitors. Talley, John J.; Getman, Daniel P.; Freskos, John N.; Lin, Ko-chung; Heintz, Robert M.; Rogier, Jr Donald J.; Bertenshaw, Deborah E. (Monsanto Co., USA). U.S. US 5475013 A **19951212**, 60 pp.
Cont.-in-part of U.S. Ser. No. 789,642, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1992-886531 19920520. PRIORITY: US 1990-615210 19901119; US 1991-789642 19911220.
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

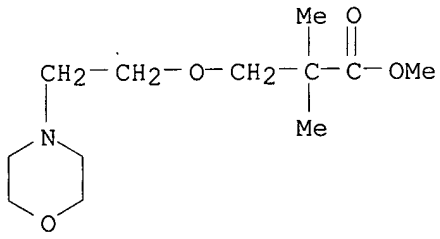
AB Urea-contg. peptide compds. I or their pharmaceutically acceptable salts, prodrugs, or esters thereof, wherein: A = radical represented by the formulas II, RR'N(CR1'R1'')qCHR1C(:Y'), III; R = e.g., H, alkoxycarbonyl, aralkoxycarbonyl; R' = e.g., H and radicals as defined for R3; q = 0, 1; R1 = e.g., H, CH2SO2NH2, CO2Me, amino acid side chains; R1', R1'' = e.g., H and radicals defined for R1; R2 = e.g., alkyl, aryl, cycloalkyl; R3 = e.g., alkyl, alkenyl, alkynyl; X' = e.g., O, CR17 where R17 = H, alkyl, and N; Y, Y', Y'' = O, S, NR15 wherein R15 = H and radicals as defined for R3; B = CR7R7'(CH2)nR8; n = 0-6; R7 and R7' = e.g., radicals as defined for R3 and amino acid side chains; R8 = e.g., CN, OH, alkyl, alkoxy; R4 = H and radicals defined by R3; R6 = H, alkyl; R20, R21, R30, R31, R32 = e.g., radicals as defined for R1; R33, R34 = e.g., H, radicals as defined for R3; are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease. Thus, e.g., Curtius rearrangement of 2,2-dimethyl-3-(4-pyridyl)propionic (prepn. given) with diphenylphosphoryl azide, followed by coupling with 3(S)-[N-(2-quinolinylcarbonyl)-L-asparaginyl]amino-2(R)-hydroxy-4-phenylbutyl-N-(4-fluorophenylmethyl)amine afforded butanediamide, N1-[3-[[[(1,1-dimethyl-2-(4-pyridyl)ethyl)amino]carbonyl](4-fluorophenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]] (IV) which inhibited HIV protease with IC50 = 4 nM.
IC ICM A61K031-47
ICS C07D215-48
NCL 514311000
CC 34-4 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 63
IT 1192-63-8P, 1-Pyrrolidinecarbonyl chloride 1619-62-1P 2049-70-9P 5324-67-4P, 2,2-Dimethyl-3-(methylsulfonyl)propionic acid 5471-77-2P 5669-14-7P, 2,2-Dimethyl-3-phenylpropionic acid 7338-27-4P, Methyl itaconate 13865-20-8P 15028-41-8P 19461-04-2P, N-Benzyl-L-phenylalanine 27943-35-7P, 2,2-Dimethyl-3-(phenylthio)propionic acid 31001-81-7P 31420-66-3P, Monoethyl trans-1,2-cyclopropanedicarboxylate 36525-60-7P, 2-(Methylsulfonylmethyl)acrylic acid 37695-38-8P 38435-02-8P, 2,2-Dimethyl-3-(phenylsulfonyl)propionic acid 38923-57-8P, Methyl 2,2-dimethyl-3-oxobutyrate 42807-45-4P 58687-28-8P 60427-77-2P 71352-14-2P 80163-58-2P 81026-69-9P 83509-04-0P 85293-46-5P 85636-56-2P 85796-30-1P 86207-79-6P 128018-43-9P 128018-44-0P 130165-86-5P 132605-93-7P 132605-97-1P 132605-98-2P 132696-45-8P 143224-45-7P 143224-62-8P 143224-63-9P 143224-64-0P 143224-65-1P 143224-66-2P 143224-67-3P 143224-69-5P 143224-70-8P 143224-71-9P 143224-72-0P 143224-73-1P 143224-74-2P 143224-75-3P 143224-76-4P 143224-77-5P 143224-78-6P 143224-79-7P 143224-80-0P 143224-81-1P 143224-82-2P 143224-83-3P 143224-84-4P 143224-85-5P

143224-86-6P 143224-87-7P 143224-89-9P 143224-90-2P 143224-91-3P
143224-92-4P 143224-93-5P 143224-94-6P, Methyl 2-
(methylsulfonylmethyl)acrylate 143224-95-7P, 2-Methyl-3-
(methylsulfonyl)propionic acid 143224-96-8P 143224-97-9P
143224-98-0P 143224-99-1P 143225-00-7P 143225-01-8P 143225-02-9P
143225-03-0P 143225-04-1P 143225-06-3P 143225-07-4P 143225-08-5P
143225-09-6P 143225-10-9P, Methyl (S)-lactate 2-methoxy-2-propyl ether
143225-11-0P 143225-13-2P 143225-15-4P 143225-16-5P 143225-17-6P
143225-18-7P 143225-22-3P 143225-23-4P 143225-26-7P 143225-27-8P
143225-28-9P 143225-31-4P 143225-32-5P 143244-71-7P 143244-72-8P
143291-14-9P 143576-87-8P 143576-88-9P 143576-90-3P 143576-91-4P
143576-93-6P 143576-94-7P 143577-08-6P 143688-40-8P 143688-41-9P,
2,2-Dimethyl-3-(4-morpholinyl)propionic acid 143688-42-0P 143688-43-1P
143688-44-2P 143688-45-3P 143688-46-4P **143688-47-5P**
143688-48-6P, 2,2-Dimethyl-3-(4-pyridyl)propionic acid 143688-49-7P,
1-(4-Pyridylmethyl)cyclopentanecarboxylic acid 143688-54-4P
143688-55-5P 143688-57-7P 143688-58-8P 143688-59-9P 143688-60-2P
143688-61-3P 149301-90-6P 149301-92-8P 149301-94-0P 149302-02-3P
149302-10-3P 158541-26-5P 174796-79-3P 174796-80-6P 174796-81-7P
174796-83-9P 174951-47-4P 174951-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(urea-contg. hydroxyethylamine peptides as retroviral protease inhibitors)

IT **143688-47-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(urea-contg. hydroxyethylamine peptides as retroviral protease inhibitors)

RN 143688-47-5 HCA

CN Propanoic acid, 2,2-dimethyl-3-[2-(4-morpholinyl)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 6 OF 29 HCA COPYRIGHT 2003 ACS on STN

122:291636 Facile synthesis and polymerization of ether substituted methacrylates. Thompson, Robert D.; Barclay, Thomas B.; Basu, Kumar R.; Mathias, Lon J. (Department Polymer Science, University Southern Mississippi, Hattiesburg, MS, 39406-0076, USA). Polymer Journal (Tokyo), 27(4), 325-38 (English) **1995**. CODEN: POLJB8. ISSN: 0032-3896. Publisher: Society of Polymer Science, Japan.

AB New difunctional methacrylate monomers contg. .beta. heteroatoms were prepd. from .alpha.-hydroxymethylacrylate esters or .alpha.-chloromethylacryloyl chloride. These monomers are more reactive than their alkane counterparts (e.g., ethacrylates), giving polymers with mol. wts. comparable to polyitaconates. This simple synthetic approach gives a wide range of difunctionalized acrylate monomers. Variations in both ester and ether substituents were explored for ease of synthesis and polymn.

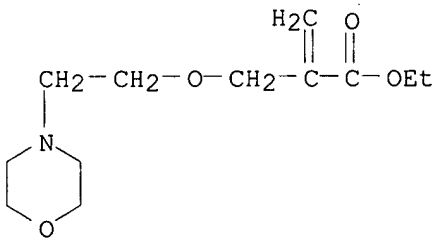
CC 35-4 (Chemistry of Synthetic High Polymers)

IT 25307-87-3P, Ethyl .alpha.-(ethoxymethyl)acrylate 25328-81-8P, Methyl .alpha.-(methoxymethyl)acrylate 153522-38-4P, Ethyl .alpha.-(methoxymethyl)acrylate 153522-39-5P, Ethyl .alpha.-(benzyloxymethyl)acrylate 163044-72-2P, Ethyl .alpha.-[(2-cyanoethoxy)methyl]acrylate 163044-73-3P, Ethyl .alpha.-[[2-(2-oxo-1-pyrrolidinyl)ethoxy]methyl]acrylate **163044-74-4P**, Ethyl .alpha.-[(2-morpholinoethoxy)methyl]acrylate 163044-75-5P, Ethyl .alpha.-[(2-phthalimidoethoxy)methyl]acrylate 163044-76-6P, tert-Butyl .alpha.-(methoxymethyl)acrylate 163044-77-7P, Benzyl .alpha.-(benzyloxymethyl)acrylate 163044-78-8P, Stearyl .alpha.-(stearyloxymethyl)acrylate 163044-79-9P, 2-Phenoxyethyl .alpha.-[(2-phenoxyethoxy)methyl]acrylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; in prepn. of alkyl (alkoxymethyl)acrylate polymers)

IT **163044-74-4P**, Ethyl .alpha.-[(2-morpholinoethoxy)methyl]acrylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; in prepn. of alkyl (alkoxymethyl)acrylate polymers)

RN 163044-74-4 HCA

CN 2-Propenoic acid, 2-[[2-(4-morpholinyl)ethoxy]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



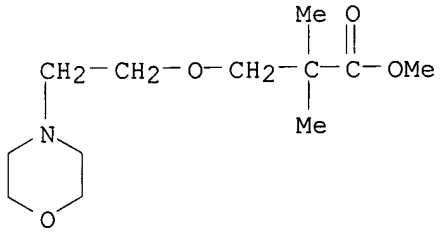
L9 ANSWER 7 OF 29 HCA COPYRIGHT 2003 ACS on STN

119:203856 Retroviral protease inhibitors. Bertenshaw, Deborah Elizabeth; Freskos, John Nicholas; Getman, Daniel Paul; Heintz, Robert Martin; Lin, Ko Chung; Rogier, Donald Joseph, Jr.; Talley, John Jeffrey (Monsanto Co., USA). PCT Int. Appl. WO 9208688 A1 **19920529**, 199 pp.
DESIGNATED STATES: W: AU, CA, CS, FI, HU, JP, KR, NO, PL, SU, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1991-US8617 19911118. PRIORITY: US 1990-615210 19901119.

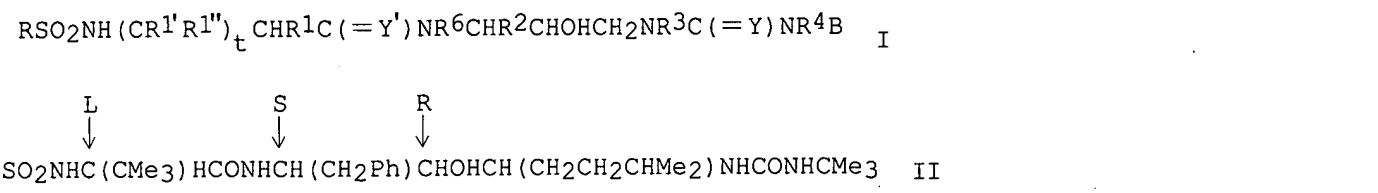
AB Urea-contg. hydroxyethylamine protease inhibitor compds. RR1NCHR2CH(OH)CH2NR3C(Z)NR4R5 (R = H, acyl; R1, R4 = H, alkyl; R2 = alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl; R3 = alkyl, alkenyl, hydroxyalkyl, cycloalkyl, cycloalkylalkyl, heterocycloalkyl, heterocycloalkylalkyl, aryl, aralkyl, heteroaralkyl; R5 = alkyl; Z = O, S) were prepd., particularly as HIV inhibitors. Thus, 2,2-dimethyl-3-(4-pyridyl)propionic acid underwent Curtius rearrangement with diphenylphosphoryl azide and Et3N in toluene and the product was treated with 3(S)-[[N-(2-quinolinylcarbonyl)-L-asparaginyl]amino]-2(R)-hydroxy-4-phenyl-N-[(4-fluorophenyl)methyl]butylamine [2-C9H6NCO-Asn-NHCH(CH2Ph)CH(OH)CH2NRCH2C6H4F-p (I, 2-C9H6N = 2-quinolinyl, R = H] to afford I [R = [[1,1-dimethyl-2-(4-pyridyl)ethyl]amino]carbonyl]. This compd. showed HIV protease inhibitory activity as follows: IC50 = 4 nM and ED50 = 37 nM.

IC ICM C07C215-48
ICS C07D295-13; C07C311-46; C07C311-47; C07C317-50; C07C323-60;

C07C275-14
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7, 15
IT 85293-46-5P 143224-94-6P 143225-21-2P 143244-74-0P
143688-47-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sapon. of)
IT **143688-47-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sapon. of)
RN 143688-47-5 HCA
CN Propanoic acid, 2,2-dimethyl-3-[2-(4-morpholinyl)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 8 OF 29 HCA COPYRIGHT 2003 ACS on STN
118:234479 Preparation of sulfonylaminoamides as HIV protease inhibitors.
Reed, Kathryn Lea; Talley, John Jeffrey (Monsanto Co., USA). PCT Int. Appl. WO 9208699 A1 **19920529**, 175 pp. DESIGNATED STATES: W: AU, CA, CS, FI, HU, JP, KR, NO, PL, SU; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1991-US8593 19911118. PRIORITY: US 1990-615210 19901119; US 1991-789645 19911114.
GI



AB Title compds. I [R = (hydroxy)alkyl, alkenyl, cycloalkyl(alkyl), heterocycloalkyl, aryl, (hetero)aralkyl; t = 0, 1; R1 = CH2SO2NH2, (cyclo)alkyl, amino acid side chains selected from asparagine, glycine, leucine, phenylalanine, alanine, etc.; R1', R1'' = H, groups defined for R1; R2 = (cyclo)alkyl, aryl, etc.; R3 = (hydroxy)alkyl, alkenyl, cycloalkyl(alkyl), heterocycloalkyl, aryl, etc.; Y, Y' = O, S; B = R5, CR7R7'(CH2)nR8; R4, R5 = groups defined for R3; NR4R5 = heterocycloalkyl, heteroaryl; R6 = H, groups defined for R3; n = 0-6; R7, R7' = groups defined for R3, amino acid side chains selected from valine, isoleucine, glycine, alanine, asparagine, etc.; CR7R7' = cycloalkyl; R8 = cyano, OH, alkoxy, (cyclo)alkyl, etc.] were prepd. as HIV protease inhibitors useful

for the treatment of AIDS. Thus, N-(n-butylsulfonyl)-L-tert-butylglycine was coupled with (2R,3R)-3-amino-1-isoamyl-1-(tert-butylcarbamoyl)amino-4-phenyl-2-butanol in the presence of hydroxybenzotriazole and Me2N(CH2)3N:C:NEt.HCl in DMF to give title compd. II. I had IC50 of 22-24 nM against HIV protease.

IC ICM C07D215-48
ICS C07D295-13; C07C311-46; C07C311-47; C07C317-50; C07C323-60; C07C275-14

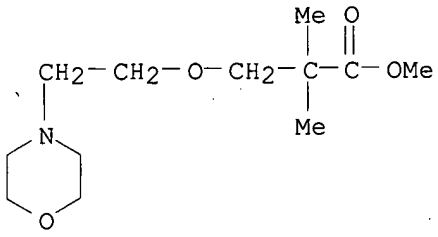
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1

IT 5324-67-4P 5471-77-2P, 2,2-Dimethylmalonate monoethyl ester 5669-14-7P, 2,2-Dimethyl-3-phenylpropionic acid 6118-13-4P 7338-27-4P, Methyl itaconate 13865-20-8P 15028-41-8P 27943-35-7P 31420-66-3P 36525-60-7P 37695-38-8P 38435-02-8P 38923-57-8P, Methyl 2,2-dimethyl-3-oxobutanoate 48162-88-5P 58687-28-8P 60427-77-2P 71352-14-2P 80163-58-2P, 2-Ethyl-2-methylmalonate monoethyl ester 81026-69-9P 83509-04-0P 85636-56-2P 86207-79-6P 98485-46-2P 128018-43-9P 128018-44-0P 130165-86-5P 132605-93-7P 132605-97-1P 132605-98-2P 132696-45-8P 133341-67-0P 143224-34-4P 143224-35-5P 143224-36-6P 143224-37-7P 143224-38-8P 143224-40-2P 143224-41-3P 143224-43-5P 143224-44-6P 143224-46-8P 143224-47-9P 143224-48-0P 143224-49-1P 143224-54-8P 143224-55-9P 143224-56-0P 143224-57-1P 143224-58-2P 143224-59-3P 143224-62-8P 143224-63-9P 143224-64-0P 143224-65-1P 143224-66-2P 143224-67-3P 143224-69-5P 143224-70-8P 143224-71-9P 143224-72-0P 143224-73-1P 143224-74-2P 143224-75-3P 143224-76-4P 143224-77-5P 143224-78-6P 143224-79-7P 143224-80-0P 143224-81-1P 143224-82-2P 143224-83-3P 143224-84-4P 143224-85-5P 143224-86-6P 143224-87-7P 143224-88-8P 143224-89-9P 143224-90-2P 143224-91-3P 143224-92-4P 143224-93-5P 143224-94-6P 143224-95-7P 143224-96-8P 143224-97-9P 143224-98-0P 143224-99-1P 143225-00-7P 143225-01-8P 143225-02-9P 143225-03-0P 143225-04-1P 143225-06-3P 143225-07-4P 143225-08-5P 143225-09-6P 143225-10-9P 143225-11-0P 143225-13-2P 143225-14-3P 143225-15-4P 143225-16-5P 143225-17-6P 143225-18-7P 143225-19-8P 143225-20-1P 143225-21-2P 143225-22-3P 143225-23-4P 143225-24-5P 143225-25-6P 143225-26-7P 143225-27-8P 143225-28-9P 143225-29-0P 143225-30-3P 143225-31-4P 143225-32-5P 143244-70-6P 143244-71-7P 143244-72-8P 143244-73-9P 143244-74-0P 143244-75-1P 143291-13-8P 143291-14-9P 143291-15-0P 143291-16-1P 143291-18-3P 143576-87-8P 143576-88-9P 143576-90-3P 143577-10-0P 143616-94-8P 143616-95-9P 143616-96-0P 143688-39-5P 143688-40-8P, Mono-tert-butyl 2,2-dimethylmalonate 143688-41-9P 143688-42-0P 143688-43-1P 143688-44-2P 143688-45-3P 143688-46-4P **143688-47-5P** 143688-48-6P 143688-49-7P 143688-50-0P 143688-51-1P 143688-52-2P 143688-53-3P 143688-54-4P 143688-55-5P 143688-56-6P 143688-57-7P 143688-58-8P 143688-59-9P 143688-60-2P 143688-61-3P 143688-62-4P 143688-63-5P 143688-64-6P 143688-65-7P 143688-66-8P 143715-16-6P 143731-19-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for HIV protease inhibitors)

IT **143688-47-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for HIV protease inhibitors)

RN 143688-47-5 HCA

CN Propanoic acid, 2,2-dimethyl-3-[2-(4-morpholinyl)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 9 OF 29 HCA COPYRIGHT 2003 ACS on STN
115:8095 Substituted tert-butyl 3-hydroxypropionates. Hickmann, Eckhard (BASF A.-G., Germany). Ger. Offen. DE 3925256 A1 **19910131**, 14 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1989-3925256 19890729.

AB R[O(CH2)2CO2CMe3]n (I; R = C2-, C3-, and C5-20-alkyl, C3-20-alkenyl, n = 1; C2-20-alkanediyl, C4-20-alkenediyl, polyether-.alpha.,.omega.-diyl, n = 2; C4-20-alkanetriyl and -tetrayl, n = 3, 4, resp.; etc.) are claimed. A method for prepg. I comprises treating ROH (same R) with CH2:CHCO2CMe3 (II) in the presence of basic catalysts. Suitable catalysts are mixt. of inorg. bases and quaternary ammonium or phosphonium compds. Thus, treating II 154 with PhCH2NMe3+ OH- 8 in EtOH 46 g gave 153.6 g EtOCH2CH2CO2CMe3. A mixt. of HOCHMeC.tplbond.CCHMeOH 114, KOH 2.8, and Bu4N+ Br- 3.2 g was added to II to give 320.8 g I (R = 1/2 CHMeC.tplbond.CCHMe, n = 2). Alkoxylation was also accomplished with Plurinol E400 or Plurinol PE 6100.

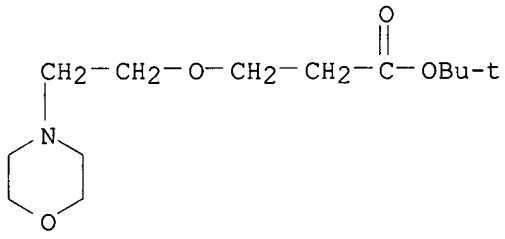
IC ICM C07C069-708
ICS C07C067-31; C07C215-06; C07C323-12; C07C255-13; C07D307-16; C07D307-46; C07D317-26; C07D261-08; C07D265-30; C07D213-55; C07D251-30
ICA C10M105-34; C10M105-56; C10M105-72; B01J031-02
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 35
IT 105-59-9DP, reaction products with tert-Bu acrylate 120-07-0DP, reaction products with tert-Bu acrylate 112032-54-9P, 1,1-Dimethylethyl 3-methoxypropionate 133717-02-9P 133759-30-5P 133803-24-4P, 1,1-Dimethylethyl 3-ethoxypropionate 133803-25-5P, 1,1-Dimethylethyl 3-(allyloxy)propionate 133803-26-6P, 1,1-Dimethylethyl 3-[2-(ethylthio)ethoxy]propionate 133803-27-7P 133803-28-8P 133803-29-9P 133803-30-2P, 1,1-Dimethylethyl 3-propoxypropionate 133803-31-3P, 1,1-Dimethylethyl 3-(1-methylethoxy)propionate 133803-32-4P, 1,1-Dimethylethyl 3-butoxypropionate 133803-33-5P 133803-34-6P 133803-35-7P, 1,1-Dimethylethyl 3-(pentyloxy)propionate 133803-36-8P 133803-37-9P 133803-38-0P 133803-39-1P, 1,1-Dimethylethyl 3-(cyclopropylmethyloxy)propionate 133803-40-4P, 1,1-Dimethylethyl 3-(cyclobutoxy)propionate 133803-41-5P, 1,1-Dimethylethyl 3-(cyclohexyloxy)propionate 133803-42-6P 133803-43-7P 133803-44-8P 133803-45-9P 133803-46-0P 133803-47-1P 133803-48-2P, 1,1-Dimethylethyl 3-(benzyloxy)propionate 133803-49-3P, 1,1-Dimthylethyl 3-(2-phenylethoxy)propionate 133803-50-6P 133803-51-7P, 1,1-Dimethylethyl 3-[(4-methoxybenzyl)oxy]propionate 133803-52-8P, 1,1-Dimethylethyl 3-[(4-nitrobenzyl)oxy]propionate 133803-53-9P 133803-54-0P 133803-55-1P, 1,1-Dimethylethyl 3-(2,2,2-trifluoroethoxy)propionate 133803-56-2P 133803-57-3P 133803-58-4P 133803-59-5P 133803-60-8P 133803-61-9P, 1,1-Dimethylethyl 3-[(2-mercaptoethyl)oxy]propionate 133803-62-0P, 1,1-Dimethylethyl 3-[2-(dimethylamino)ethoxy]propionate 133803-63-1P, 1,1-Dimethylethyl 3-[3-(dimethylamino)propoxy]propionate 133803-64-2P 133803-65-3P 133803-66-4P 133803-67-5P 133803-68-6P 133803-69-7P

133803-70-0P 133803-71-1P 133803-72-2P **133803-73-3P**
133803-74-4P 133803-75-5P 133803-76-6P 133803-77-7P 133803-78-8P
133803-79-9P 133803-80-2P 133803-81-3P 133803-82-4P 133803-86-8P
133803-87-9P 133803-88-0P 133823-65-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **133803-73-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 133803-73-3 HCA

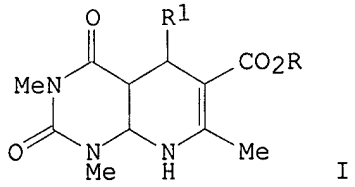
CN Propanoic acid, 3-[2-(4-morpholinyl)ethoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 10 OF 29 HCA COPYRIGHT 2003 ACS on STN

114:207192 The Hantzsch synthesis with 6-aminouracils: one step synthesis of pyrido[2,3-d]pyrimidines. Kajino, Masahiro; Meguro, Kanji (Res. Dev. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan). Heterocycles, 31(12), 2153-61 (English) **1990**. CODEN: HTCYAM. ISSN: 0385-5414. OTHER SOURCES: CASREACT 114:207192.

GI



I

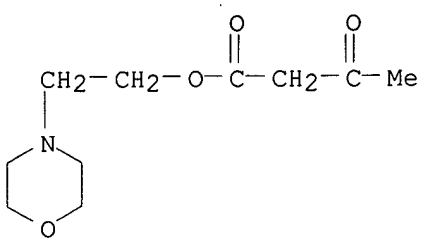
AB A one-step synthesis of a new pyrido[2,3-d]pyrimidine derivs., e.g. I [R = Me, Et, (CH2)2NMeCH2Ph, (CH2)2NMePh, R1 = C6H4NO2-3, C6H3Cl2-2,3], was achieved through the Hantzsch synthesis using 6-aminouracils as enamine nucleophiles. Antihypertensive activity of I was evaluated.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

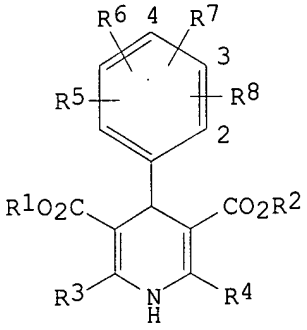
IT 89-98-5, 2-Chlorobenzaldehyde 99-61-6, 3-Nitrobenzaldehyde 105-45-3 120-14-9, 3,4-Dimethoxybenzaldehyde 141-97-9 459-57-4, 4-Fluorobenzaldehyde 2043-61-0, Cyclohexanecarboxaldehyde 6334-18-5, 2,3-Dichlorobenzaldehyde 32863-32-4, 4-Benzofurazancarboxaldehyde **50899-08-6** 54527-65-0 54527-66-1 89226-49-3 90096-30-3 133657-28-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in synthesis of pyridopyrimidine)

IT **50899-08-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in synthesis of pyridopyrimidine)

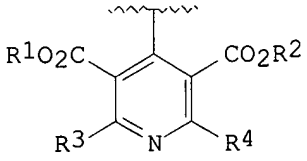
RN 50899-08-6 HCA
CN Butanoic acid, 3-oxo-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 11 OF 29 HCA COPYRIGHT 2003 ACS on STN
113:78379 Preparation of methylenedioxyphenylpyridinedicarboxylic acid esters for treatment and prevention of liver diseases. Iwamoto, Hidenori; Koide, Tokuo; Matsuhisa, Akira; Ikadai, Hiroyuki (Yamanouchi Pharmaceutical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 02069475 A2 **19900308** Heisei, 18 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1988-223335 19880905.
GI



I



II

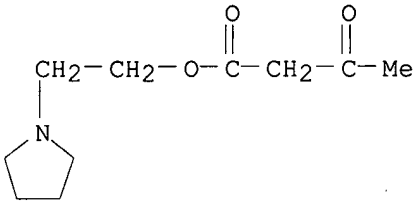
AB The title compds. [I; II; R1, R2 = alkyl; or one of R1 and R2 = alkyl and the other = ZNR9R10; Z = alkylene; R9, R10 = alkyl or NR9R10 forming 5- or 6-membered ring; R3, R4 = alkyl; or one of R3 and R4 = alkyl and the other = Z1R11; Z1 = alkylene; R11 = dialkylamine, 4-alkylpiperadino, pyridylthio, mono- or dialkylaminoalkylthio; R5, R6 = H, alkoxy, COH, (un)substituted CO2H or CONH2; R7R8 = alkylenedioxy] are prepd. Thus, I (R1 = R2 = R3 = R4 = Me, R5 = CO2Me, R6 = H, R7R8 = 3,4-OCH2O) was stirred with pyridinium bromide perbromide in CHCl3-pyridine for 30 min at 0.degree. and the product was reacted with Me2NH.HCl in CHCl3 contg. Et3N for 1 h at room temp. to give I.HCl (R1 = R2 = R3 = Me, R4 = CH2NMe2, R5 = CO2Me, R6 = H, R7R8 = 3,4-OCH2O) (III). A total of 29 I and II were prepd. and III in vivo at 10 mg/kg/5 mol p.o. in rats inhibited 91.7% the effect of D-galactosamine on livers. Capsules contg. III were formulated.
IC ICM C07D405-04
ICS C07D405-04; C07D405-14
ICA A61K031-44; A61K031-495; C07D471-04; C07D491-056
CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 63
IT 6131-49-3 **55985-43-8**, 2-Pyrrolidinoethyl acetoacetate

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with methylenedioxybenzaldehyde and Me aminocrotonate)

IT **55985-43-8**, 2-Pyrrolidinoethyl acetoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with methylenedioxybenzaldehyde and Me aminocrotonate)

RN 55985-43-8 HCA

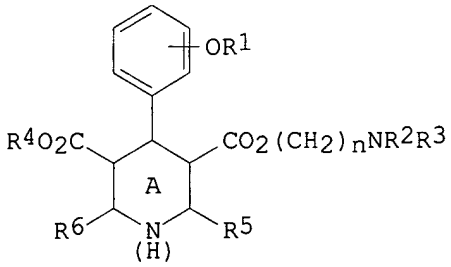
CN Butanoic acid, 3-oxo-, 2-(1-pyrrolidinyl)ethyl ester (9CI) (CA INDEX NAME)



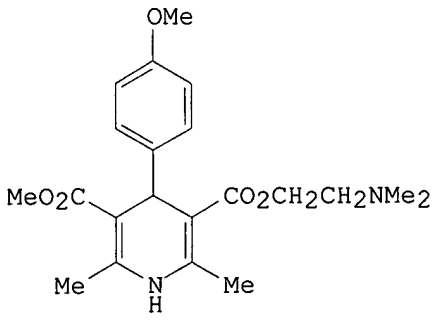
L9 ANSWER 12 OF 29 HCA COPYRIGHT 2003 ACS on STN

113:78172 Dihydropyridine and pyridine derivatives as drugs for treatment of liver disease and their preparation. Iwamoto, Hidenori; Koide, Tokuo; Matsuhisa, Akira; Ikadai, Hiroyuki (Yamanouchi Pharmaceutical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 02069459 A2 **19900308** Heisei, 15 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1988-220624 19880902.

GI



I



II

AB The title compds. I (R1 = alkyl; R2, R3 = alkyl; or 1 of R2, R3 is alkyland the other is PhCH2; or NR2R3 = 5- or 6-membered ring; R4 = alkyl; R5, R6 = alkyl; or 1 of R5, R6 is alkyl and the other is alkylaminoalkyl;

n = 2-5; ring A is dihydropyridine, pyridine) were prepd. A mixt. of p-anisaldehyde and 2-dimethylaminoethyl acetoacetate in benzene contg. AcOH and piperidine was refluxed for 2 h to give, after workup and evapn. of benzene, a residue, which was condensed with Me 3-aminocrotonate in isopropanol to give dihydropyridine II. II at 10 mg/kg orally inhibited the increase of serum GPT in D-galactosamine-treated rats by 61.1%.

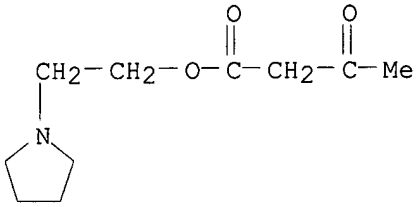
IC ICM C07D211-90
ICS A61K031-44; A61K031-445; C07D213-80

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT 123-11-5, reactions 135-02-4, o-Anisaldehyde 591-31-1, m-Anisaldehyde 4278-29-9, Acetoacetic acid (2-diethylamino)ethyl ester 6131-49-3, Acetoacetic acid (2-dimethylamino)ethyl ester 14205-39-1, Methyl 3-aminocrotonate 54527-65-0, 1-(2-N-Benzyl-N-methylaminoethyl)acetoacetate **55985-43-8** 71784-33-3, 1-(3-Dimethylaminopropyl)acetoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in prepn. of dihydropyridine and pyridine derivs. for treating liver disease)

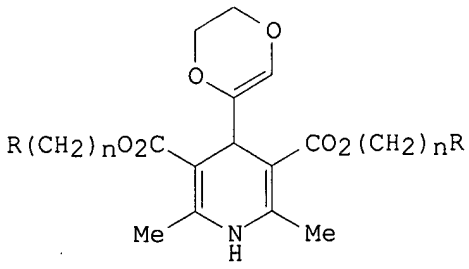
IT **55985-43-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in prepn. of dihydropyridine and pyridine derivs. for treating liver disease)

RN 55985-43-8 HCA
CN Butanoic acid, 3-oxo-, 2-(1-pyrrolidinyl)ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 13 OF 29 HCA COPYRIGHT 2003 ACS on STN
113:40701 4-[2-(5,6-Dihydro-p-dioxinyl)]-2,6-dimethyl-1,4-dihydropyridine-3,5-carboxylic acid diesters as antitumor synergists. Suzuki, Kenichi; Inada, Haruaki; Kigami, Akira; Sano, Tetsuro (Nikken Chemicals Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 02040383 A2 **19900209** Heisei, 8 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1988-186711 19880728.

GI



I

AB The title compds. I (R = pyridyl which may have 1 Me or Et, morpholino, NMeCH2Ph; n = 1-4), useful as antitumor agents showing enhanced activity in combination with other antitumor agents, were prepd. I have no Ca2+ pass-blocking activity, thus give no damage to a cardiovascular system. A mixt. of 2-formyl-p-dioxene, 3-(3-pyridyl)propyl acetoacetate, an aq. NH3 soln., and Me2CHOH was refluxed for 20 h to give 13.2% I (R = 3-pyridyl, n = 3) (II). A combined application of 100 mg/kg II with 30 .mu.g/kg vincristine (III) to mice bearing III-resistant leukemia cell P388/VCR enhanced antitumor activity at a ratio of increased life span to III alone 130%, vs. 130% for Verapamil. II at 10-7 M inhibited the K+-induced contraction of rat rectum with a rate of 4.2% vs. 50.2% for Verapamil.

IC ICM C07D405-04
ICS C07D405-14

ICA A61K031-435; A61K031-44

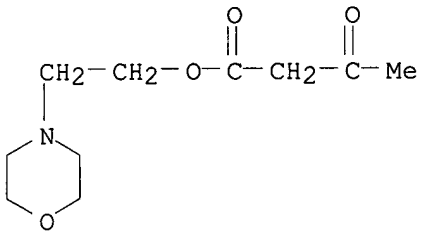
CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 50899-06-4, 2-Pyridylmethyl acetoacetate **50899-08-6** 54527-65-0
56019-57-9 103839-99-2 127955-98-0 127955-99-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with formyldioxene and ammonia, in prepn. of antitumor synergist)

IT **50899-08-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with formyldioxene and ammonia, in prepn. of antitumor synergist)

RN 50899-08-6 HCA

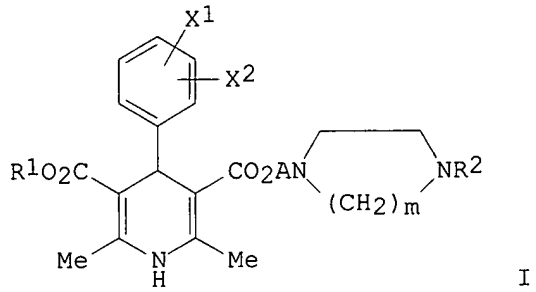
CN Butanoic acid, 3-oxo-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)



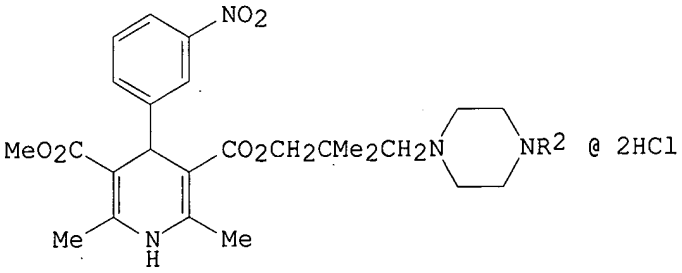
L9 ANSWER 14 OF 29 HCA COPYRIGHT 2003 ACS on STN

111:23532 Preparation of 1,4-dihydropyridine derivatives as calcium antagonists. Matsui, Hiroshi; Fukada, Fumio; Mori, Takayoshi; Kakeya, Senji; Kitao, Kazuhiko (Kyoto Pharmaceutical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 63225355 A2 **19880920** Showa, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1987-57717 19870312.

GI



I



II

AB The title compds. [I; X1, X2 = H, FCH2, FCH2O, halo, cyano, NO2; R1 = alkyl; R2 = acyl, alkoxycarbonyl, acylalkyl, etc.; A = (substituted) alkylene having .gtoreq.5 C atoms; m = 1-3], effective Ca antagonists, are prepd. Allyl chloride and Et3N added to a soln. of II (R2 = H) in THF and stirred at 50.degree. to give 75% allyl deriv. II (R2 = allyl), which lowered the blood pressure by 81 and 104 mmHg after 4 and 8 h, resp., at 10 mg/kg p.o. in rats. A capsule formulation contg. I 5, lactose 100, poly(vinylpyrrolidone) 3, and stearic acid 2 mg was prepd.

IC ICM C07D211-90
ICS A61K031-455

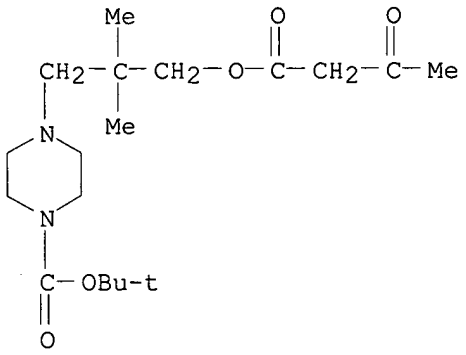
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT 119687-29-5P 119700-51-5P 119700-52-6P 119700-53-7P 119700-54-8P **119700-55-9P 119700-56-0P** 119700-57-1P 119700-58-2P **119700-59-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of calcium antagonists)

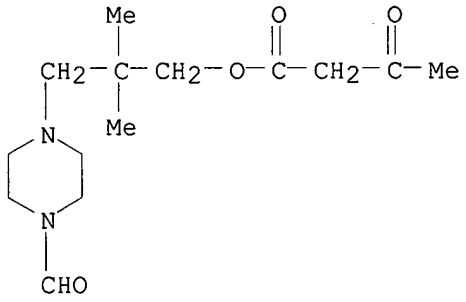
IT **119700-55-9P 119700-56-0P 119700-59-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of calcium antagonists)

RN 119700-55-9 HCA

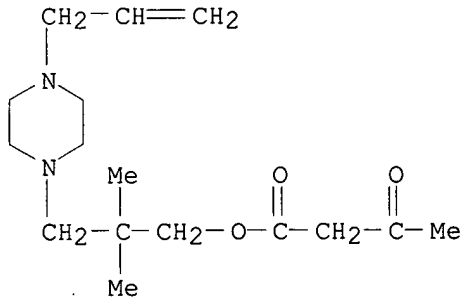
CN 1-Piperazinecarboxylic acid, 4-[3-(1,3-dioxobutoxy)-2,2-dimethylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



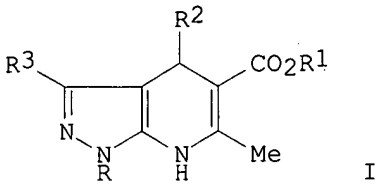
RN 119700-56-0 HCA
CN Butanoic acid, 3-oxo-, 3-(4-formyl-1-piperazinyl)-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)



RN 119700-59-3 HCA
CN Butanoic acid, 3-oxo-, 2,2-dimethyl-3-[4-(2-propenyl)-1-piperazinyl]propyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 15 OF 29 HCA COPYRIGHT 2003 ACS on STN
110:95080 Studies on dihydropyridines. II. Synthesis of 4,7-dihydropyrazolo[3,4-b]pyridines with vasodilating and antihypertensive activities. Adachi, Ikuo; Yamamori, Teruo; Hiramatsu, Yoshiharu; Sakai, Katsunori; Sato, Hatsuo; Kawakami, Masaru; Uno, Osamu; Ueda, Motohiko (Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan). Chemical & Pharmaceutical Bulletin, 35(8), 3235-52 (English) **1987**.
CODEN: CPBTAL. ISSN: 0009-2363. OTHER SOURCES: CASREACT 110:95080.
GI



I

AB A series of 4-aryl-4,7-dihydropyrazolo[3,4-b]pyridine-5-carboxylate derivs. I (R = Me, Ph, cyclopentyl; R1 = Me, Et, CHMe2, cyclohexyl, substituted phenethyl, etc.; R2 = 2-O2NC6H4, 3-O2NC6H4, 2-ClC6H4, 2.8-Cl2C6H4, pyridyl; R3 = H, Me, CHMe2, Ph, cycloalkyl, CO2Et, pyridyl, etc.) was prepd. and the compds. were tested for Ca-blocking activity in isolated guinea pig portal vein, antihypertensive activity in spontaneously hypertensive rats, and coronary vasodilating effect in isolated guinea pig heart. A no. of derivs. had potent antihypertensive and coronary vasodilating activities. The structure-activity relationships of the series indicated that a 3-cyclopentyl or 3-cyclohexyl substituent and a hydrophobic 5-ester moiety with moderate bulkiness were effective for increasing the pharmacol. potencies.

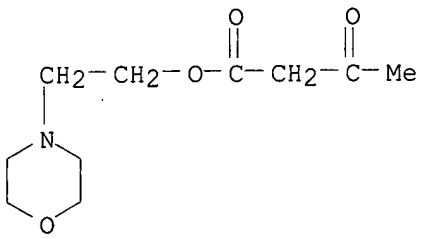
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 105-45-3, Methyl acetoacetate 141-97-9, Ethyl acetoacetate 542-08-5 6624-84-6, Pentyl acetoacetate 6947-02-0, Cyclohexyl acetoacetate 24370-84-1, Phenethyl acetoacetate **50899-08-6** 57582-44-2, 2-Phenoxyethyl acetoacetate 71784-33-3 90252-74-7, 2-(Methylthio)ethyl acetoacetate 91599-98-3 98291-22-6 100287-89-6 100287-90-9 100303-68-2, 2-(4-Chlorophenyl)ethyl acetoacetate 100303-69-3, 2-(3,4-Dimethoxyphenyl)ethyl acetoacetate 100303-72-8, 2-(Phenylthio)ethyl acetoacetate 100303-73-9 100303-74-0 100303-75-1 118431-93-9, 2-(4-Bromophenyl)ethyl acetoacetate 118431-94-0 118431-95-1 118447-45-3, 2-(3-Trifluoromethylphenyl)ethyl acetoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with nitrobenzaldehydes)

IT **50899-08-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with nitrobenzaldehydes)

RN 50899-08-6 HCA

CN Butanoic acid, 3-oxo-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)

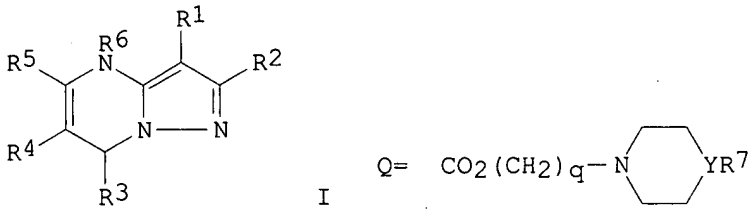


L9 ANSWER 16 OF 29 HCA COPYRIGHT 2003 ACS on STN

109:149558 Preparation of 4,7-dihydropyrazolo[1,5-a]pyrimidine derivatives as calcium antagonists. (Yoshitomi Pharmaceutical Industries, Ltd., Japan).

Jpn. Kokai Tokkyo Koho JP 63060985 A2 **19880317** Showa, 39 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1987-198872 19870807. PRIORITY: CA 1986-515584 19860808.

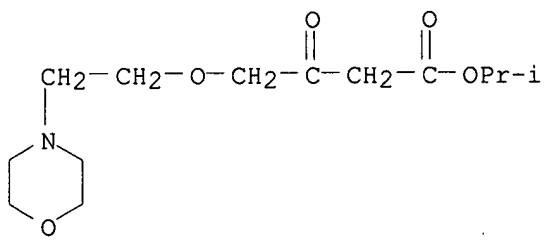
GI



I

AB The title compds. [I; R1 = CHO, PhCO, C1-8 alkanoyl; R2 = H, halo, NO2, NH2, acylamino, C1-8 alkyl, C3-8 cycloalkyl, cyano, CO2H, CONH2, CHO, etc.; R3 = H, C1-8 alkyl, C2-10 alkenyl, C2-10 alkynyl, (un)substituted aryl, (un)substituted Ph, etc.; R4 = H, NO2, cyano, acyl, (mono- or disubstituted) CONH2 or C(S)NH2, (unsubstituted CO2H; R5 = H, cyano, C1-8 alkyl, haloalkyl, hydroxyalkyl, aminoalkyl, CHO, NH2, (un)substituted Ph or aralkyl, etc.; R6 = H, C1-8 alkyl, haloalkyl, hydroxyalkyl, aminoalkyl, acyl, heteroaryl, (un)substituted aralkyl], having Ca antagonist or Ca agonist/antagonist activities (no data) and useful as, e.g. antihypertensives, were prepd. A soln. of 3.0 4-[2-(phthalimido)ethoxy]-3-oxobutyric acid iso-Pr ester (II) (prepn. given) and 1.5 g 2,3-F2C6H3CHO in benzene contg. 2 drops each of AcOH and piperidine was refluxed for 3 h with removal of H2O by a Dean-Stark trap. After removing the solvent, 1.1 g 3-amino-4-cyanopyrazole and 10 mL DMF was added to the residue and the mixt. was heated at 100.degree. for 6 h to give 1.65 g I [R1 = cyano, R2 = R6 = H, R3 = 2,3-F2C6H3, R4 = CO2CHMe2, R5 = 2-(phthalimido)ethoxy] which was treated with H2NNH2.H2O in MeOH-CHCl3 at 50.degree. for 5 h to give, after conversion into a HCl salt, I (R5 = H2NCH2CH2O, R1-R4,R6 as defined above).HCl.

IC ICM C07D487-04
ICA A61K031-505
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT 88150-69-0P 112641-83-5P 116646-20-9P 116646-21-0P 116646-22-1P 116646-23-2P **116646-24-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with benzaldehyde deriv.)
IT **116646-24-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with benzaldehyde deriv.)
RN 116646-24-3 HCA
CN Butanoic acid, 4-[2-(4-morpholinyl)ethoxy]-3-oxo-, 1-methylethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 17 OF 29 HCA COPYRIGHT 2003 ACS on STN
107:192961 Repellent effect of Mannich bases derived from lactic acid esters. Kovalenko, L. G.; Ruban, E. M.; Skrynik, E. M.; Viktorov-Nabokov, O. V.; Korneeva, L. A.; Dremova, V. P.; Markina, V. V. (Kiev. Gos. Univ., Kiev, USSR). Meditsinskaya Parazitologiya i Parazitarnye Bolezni (1), 44-8 (Russian) **1987**. CODEN: MPPBAB. ISSN: 0025-8326.

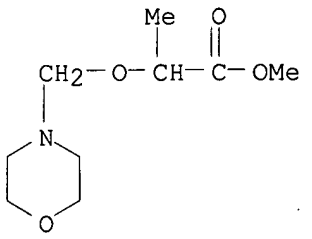
AB O-Aminomethylation of lactic acid esters gave 30 MeHCO2ROCH2NR1R2, I (R = Me, Pr, iso-Pr, Bu, isoBu, C5H11, isoC5H11; NR1R2 = diethylamino, dibutylamino, benzylamino, morpholino, or piperidino). Coeff. of Aedes aegypti repellency by I was 10-100% and the protection persisted for 0-31 days. These parameters were 30-100% and 0-30 days, resp., for the fleas Xenopsylla cheopis, Ceratophyllus sciurorum, and C. consimilis. Lactic acid O-(N-benzylaminomethyl) isoamylate and lactic acid O-(N-benzylaminomethyl) isobutylate were tested in the field against A. communis and A. vexans and the persistence of their action exceeded that of the DETA std. by 3-6 days, while the repellency was equal.

CC 5-4 (Agrochemical Bioregulators)

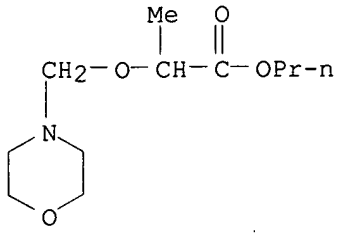
IT **111181-74-9P** 111181-75-0P 111181-76-1P 111181-77-2P
111181-78-3P 111181-79-4P 111181-80-7P 111181-81-8P
111181-82-9P 111181-83-0P 111181-84-1P 111181-85-2P
111181-86-3P 111181-87-4P 111181-88-5P 111181-89-6P
111181-90-9P 111181-91-0P 111181-92-1P 111181-93-2P
111181-94-3P 111181-95-4P 111181-96-5P 111181-97-6P
111181-98-7P 111181-99-8P **111182-00-4P** 111182-01-5P
111182-02-6P 111182-03-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and insect-repellent activity of)

IT **111181-74-9P 111181-78-3P 111181-82-9P**
111181-90-9P 111181-94-3P 111181-98-7P
111182-00-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and insect-repellent activity of)

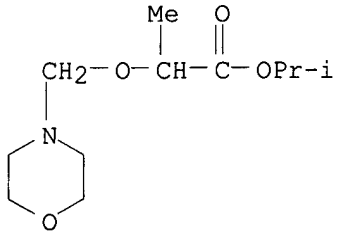
RN 111181-74-9 HCA
CN Propanoic acid, 2-(4-morpholinylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)



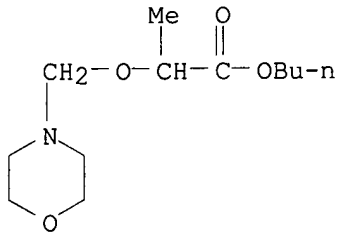
RN 111181-78-3 HCA
CN Propanoic acid, 2-(4-morpholinylmethoxy)-, propyl ester (9CI) (CA INDEX NAME)



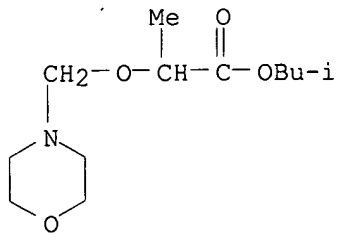
RN 111181-82-9 HCA
CN Propanoic acid, 2-(4-morpholinylmethoxy)-, 1-methylethyl ester (9CI) (CA INDEX NAME)



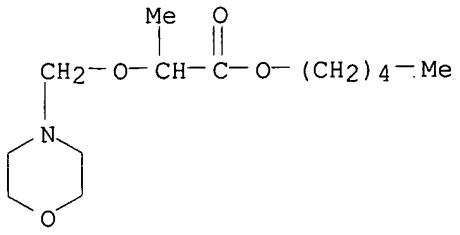
RN 111181-90-9 HCA
CN Propanoic acid, 2-(4-morpholinylmethoxy)-, butyl ester (9CI) (CA INDEX NAME)



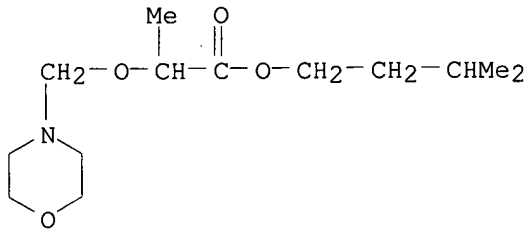
RN 111181-94-3 HCA
CN Propanoic acid, 2-(4-morpholinylmethoxy)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



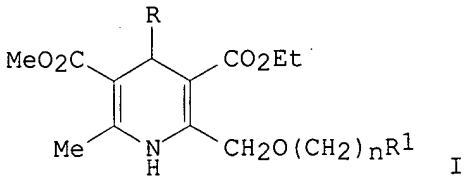
RN 111181-98-7 HCA
CN Propanoic acid, 2-(4-morpholinylmethoxy)-, pentyl ester (9CI) (CA INDEX NAME)



RN 111182-00-4 HCA
CN Propanoic acid, 2-(4-morpholinylmethoxy)-, 3-methylbutyl ester (9CI) (CA INDEX NAME)



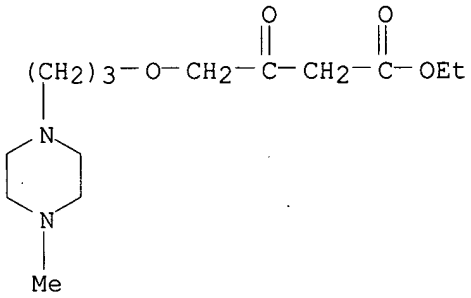
L9 ANSWER 18 OF 29 HCA COPYRIGHT 2003 ACS on STN
105:172250 Long-acting dihydropyridine calcium antagonists. 1. 2-Alkoxymethyl derivatives incorporating basic substituents. Arrowsmith, John E.; Campbell, Simon F.; Cross, Peter E.; Stubbs, John K.; Burges, Roger A.; Gardiner, Donald G.; Blackburn, Kenneth J. (Pfizer Cent. Res., Sandwich/Kent, CT13 9NJ, UK). Journal of Medicinal Chemistry, 29(9), 1696-702 (English) **1986**. CODEN: JMCMAR. ISSN: 0022-2623.
OTHER SOURCES: CASREACT 105:172250.
GI



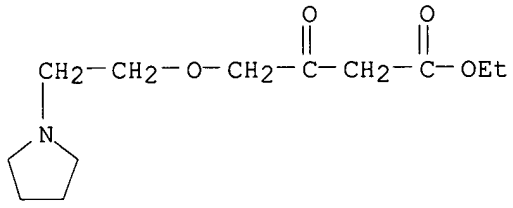
I

AB Aminoalkoxymethyldihydropyridines I [R = Ph, substituted Ph, 1-naphthyl, 2-thienyl, 4-pyridyl; R1 = (un)substituted NH2; n = 2, 3] were prepd. from RCHO, R1(CH2)nOCH2COCH2CO2Et, and H2NCMe:CHCO2Me or via I (R = N3, phthalimido). Their potencies as Ca antagonists were detd. I (R = 2-ClC6H4, R1 = NH2, n = 2) (amlodipine) was comparable in potency to nifedipine and had an elimination half-life of 30 h in dogs. Oral bioavailability approached 100%, and hemodynamic responses were gradual in onset and long-lasting in effect. The two enantiomers were prepd.; the bulk of the activity resided with the (-)-isomer. X-ray crystallog. studies, carried out on I (R = 2-ClC6H4, R = morpholinosulfonyl, n = 2) suggest the existence of a weak H bond between the side-chain O and the H

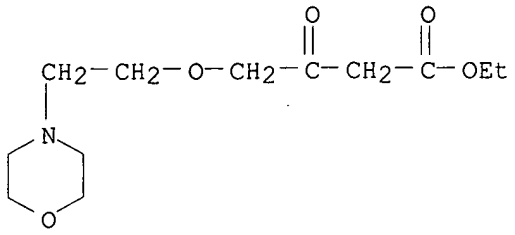
on the ring N.
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT **109788-89-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with chlorobenzylidenemalonate and ammonium acetate)
IT 84157-65-3 88150-45-2 88150-69-0 88150-75-8 **103069-56-3** **103069-57-4 103069-58-5 103069-59-6** 103069-60-9 103069-61-0 103069-62-1 **103069-63-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aldehydes and aminocrotonate or arylideneacetoacetate)
IT **109788-89-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with chlorobenzylidenemalonate and ammonium acetate)
RN 109788-89-8 HCA
CN Butanoic acid, 4-[3-(4-methyl-1-piperazinyl)propoxy]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



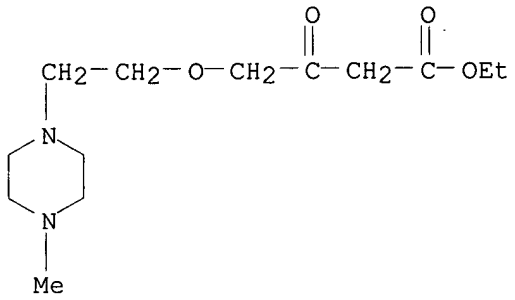
IT **103069-56-3 103069-57-4 103069-58-5 103069-59-6 103069-63-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aldehydes and aminocrotonate or arylideneacetoacetate)
RN 103069-56-3 HCA
CN Butanoic acid, 3-oxo-4-[2-(1-pyrrolidinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)



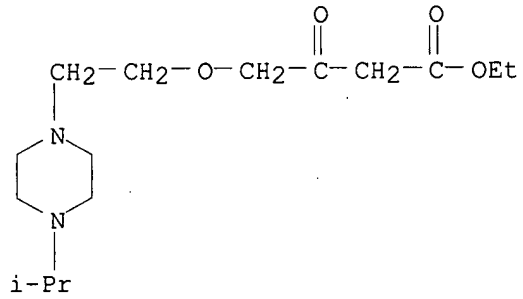
RN 103069-57-4 HCA
CN Butanoic acid, 4-[2-(4-morpholinyl)ethoxy]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



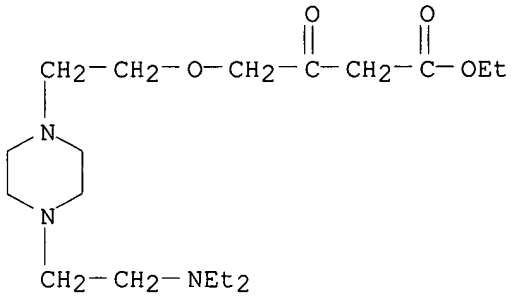
RN 103069-58-5 HCA
CN Butanoic acid, 4-[2-(4-methyl-1-piperazinyl)ethoxy]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



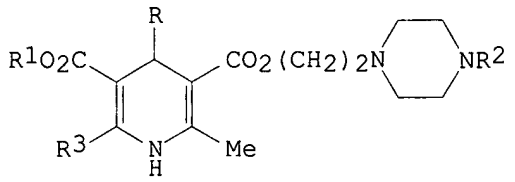
RN 103069-59-6 HCA
CN Butanoic acid, 4-[2-[4-(1-methylethyl)-1-piperazinyl]ethoxy]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 103069-63-2 HCA
CN Butanoic acid, 4-[2-[4-[2-(diethylamino)ethyl]-1-piperazinyl]ethoxy]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



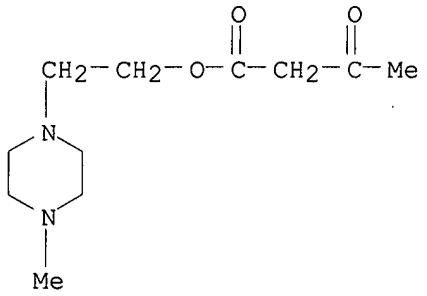
L9 ANSWER 19 OF 29 HCA COPYRIGHT 2003 ACS on STN
105:133842 New 1,4-dihydropyridine derivatives with potent and long-lasting hypotensive effect. Meguro, Kanji; Aizawa, Masahiro; Sohda, Takashi; Kawamatsu, Yutaka; Nagaoka, Akinobu (Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan). Chemical & Pharmaceutical Bulletin, 33(9), 3787-97 (English) **1985**. CODEN: CPBTAL. ISSN: 0009-2363. OTHER SOURCES: CASREACT 105:133842.
GI



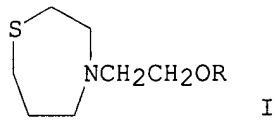
I

AB Piperazinylalkyl esters I (R = substituted Ph, R1 = Me, Et; R2 = Ph2CH, Ph, substituted Ph; R3 = Me, NH2), bearing a lipophilic substituent on the 4-nitrogen of the piperazine ring, were prepd. and tested for hypotensive effect in spontaneously hypertensive rats. I having a diphenylmethyl moiety on the piperazine ring showed extremely potent and long-lasting hypotensive properties. Analogs related to I, generally including R = 3-O2NC6H4, were also prepd., and the structure-activity relationships are discussed.
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 27
IT 89226-49-3P 90096-13-2P 90096-14-3P 90096-15-4P 90096-16-5P
90096-18-7P 90096-19-8P 90096-20-1P 90096-21-2P 90096-25-6P
90096-26-7P 90096-27-8P 90096-28-9P 90096-29-0P 90096-30-3P
90096-31-4P 90096-32-5P 97795-54-5P **104305-97-7P**
104329-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with arom. aldehyde and aminocrotonate, piperazinylethylpyridinedicarboxylate from)
IT **104305-97-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with arom. aldehyde and aminocrotonate,

piperazinylethylpyridinedicarboxylate from)
RN 104305-97-7 HCA
CN Butanoic acid, 3-oxo-, 2-(4-methyl-1-piperazinyl)ethyl ester (9CI) (CA INDEX NAME)

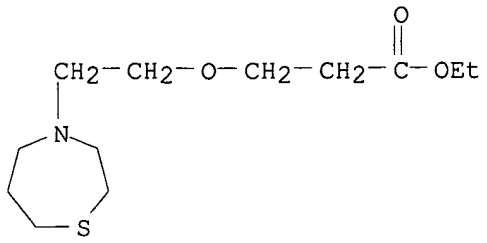


L9 ANSWER 20 OF 29 HCA COPYRIGHT 2003 ACS on STN
99:5608 Perhydro-1,4-thiazepine derivatives with expected pharmacological activity. Part II. 2-(Perhydro-1,4-thiazepin-4-yl)ethyl benzyl and benzhydryl ethers with mycostatic and anthelmintic activity. Strzelczyk, Marek (Dep. Gen. Chem. Physiol. Biochem., Military Med. Acad., Lodz, 90-647, Pol.). Polish Journal of Pharmacology and Pharmacy, Volume Date 1982, 34(4), 265-73 (English) **1983**. CODEN: PJPPAA. ISSN: 0301-0244. OTHER SOURCES: CASREACT 99:5608.
GI

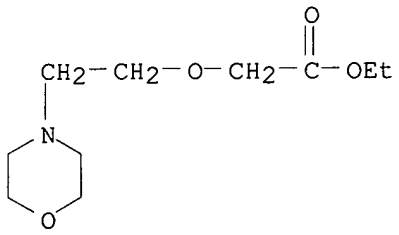


I

AB Title ethers I [R = PhCH2, PhOCH2CH2, 2,4-Cl2C6H3CH2, 2-BrC6H4CH2, Ph2CH, 4-ClC6H4CHPh, EtO2CCH2CH2] were prepd. by etherification of 4-(2-hydroxy- or 2-chloroethyl)perhydro-1,4-thiazepine. I (R = PhOCH2CH2 or 2-BrC6H4CH2) showed the highest mycostatic and anthelmintic activities. Spectral data are given.
CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 5
IT 86010-75-5P 86010-76-6P 86010-77-7P 86010-78-8P 86010-79-9P 86010-80-2P **86010-81-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra, and anthelmintic activities of)
IT **86010-81-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra, and anthelmintic activities of)
RN 86010-81-3 HCA
CN Propanoic acid, 3-[2-(tetrahydro-1,4-thiazepin-4(5H)-yl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

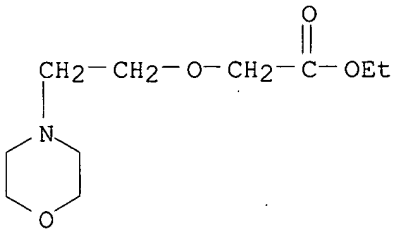


L9 ANSWER 21 OF 29 HCA COPYRIGHT 2003 ACS on STN
96:162113 Oxaalkanoate anti-ulcer compounds. Brown, James P.; Laughlin, Robert G. (Procter and Gamble Co., USA). U.S. US 4314060 A **19820202**, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1979-57923 19790716.
AB RN+R1R2[(CH2)nO]m(CH2)pCO2- (R = C11-30 alkyl; R1, R2 = Me, Et, Pr; n = 2, 3; m = 1, 2, 3; p = 1, 2) were prepd. as antiulcer drugs. Thus, Me2NCH2CH2OCH2CH2CN was treated with EtOH and the resulting esters treated with docosyl bromide to give Me(CH)21N+Me2CH2CH2OCH2CH2CO2Et Br- which was treated with carbonate to give Me(CH2)21N+Me2CH2CH2OCH2CH2CO2-. At 100 mg/kg Me(CH2)13N+Me2(CH2CH2O)3CH2CO2- reduced ulcer incidence by 75% in the Shay Rat test system.
IC C07D295-14; C07C101-18; C07C101-12
NCL 544171000
CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 1, 63
IT **78546-50-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and reaction with docosyl iodide)
IT **78546-50-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and reaction with docosyl iodide)
RN 78546-50-6 HCA
CN Acetic acid, [2-(4-morpholinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

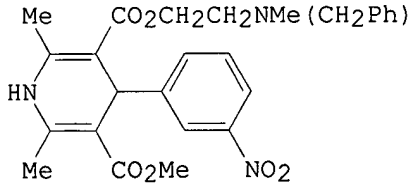


L9 ANSWER 22 OF 29 HCA COPYRIGHT 2003 ACS on STN
95:80179 Oxaalkanoate antiulcer composition. Laughlin, Robert G.; Fu, Juian-Juian L. (Procter and Gamble Co., USA). U.S. US 4263281 **19810421**, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1979-57922 19790716.
AB Zwitterionic compds. R3N+ZCO2- (at least one R group is a lipophilic hydrocarbyl group contg. >10 C atoms and the remainder are hydrocarbyl contg. <10 C atoms; Z = oxyalkylene with a chain length of .ltoreq.11 total atoms), useful in the prevention or treatment of ulcers, were prepd. Thus, Me2NCH2CH2OCH2CH2CN was converted to Me(CH2)21N+Me2CH2CH2OCH2CH2CO2-

via Me2NCH2CH2OCH2CH2CO2Et and Me(CH2)21N+Me2CH2CH2OCH2CH2CO2Et Br-.
IC A61K033-00; A61K033-12; A61K033-08; A61K031-205
NCL 424155000
CC 23-16 (Aliphatic Compounds)
Section cross-reference(s): 63
IT 78546-44-8P 78546-47-1P **78546-50-6P** 78546-53-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and quaternization of)
IT **78546-50-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and quaternization of)
RN 78546-50-6 HCA
CN Acetic acid, [2-(4-morpholinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)



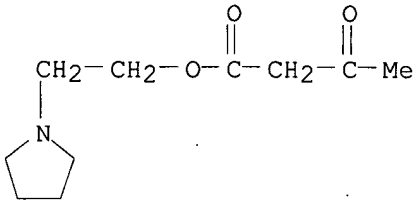
L9 ANSWER 23 OF 29 HCA COPYRIGHT 2003 ACS on STN
91:193122 Synthesis of new water-soluble dihydropyridine vasodilators.
Iwanami, Masaru; Shibanuma, Tadao; Fujimoto, Masaharu; Kawai, Ryutaro; Tamazawa, Kazuharu; Takenaka, Toichi; Takahashi, Kozo; Murakami, Masuo (Cent. Res. Lab., Yamanouchi Pharm. Co., Ltd., Tokyo, 174, Japan).
Chemical & Pharmaceutical Bulletin, 27(6), 1426-40 (English) **1979**. CODEN: CPBTAL. ISSN: 0009-2363.
GI



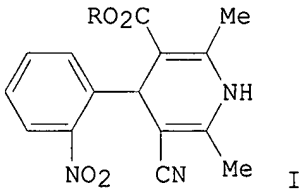
I

AB Several kinds of water-sol. dihydropyridine vasodilators were prepd. and their vasodilating activities were evaluated. Among them I.HCl has outstanding activity and bioavailability. Various synthetic routes for this compd. were examd.
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT 99-61-6 141-97-9 459-73-4 623-33-6 6131-49-3 7318-00-5
14205-39-1 14205-43-7 14205-46-0 24370-84-1 39562-61-3
43107-09-1 43107-11-5 52937-90-3 54527-65-0 54527-67-2
54527-68-3 54527-69-4 54527-70-7 54527-73-0 54527-74-1

55985-43-8 55985-44-9 56019-57-9 71784-30-0 71784-31-1
71784-32-2 71784-33-3 71784-37-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(Hantzch reaction of)
IT **55985-43-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Hantzch reaction of)
RN 55985-43-8 HCA
CN Butanoic acid, 3-oxo-, 2-(1-pyrrolidinyl)ethyl ester (9CI) (CA INDEX NAME)

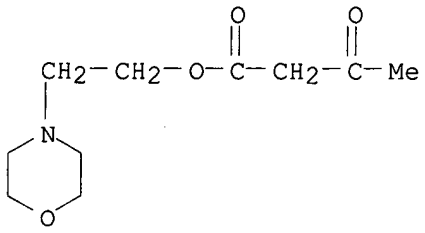


L9 ANSWER 24 OF 29 HCA COPYRIGHT 2003 ACS on STN
90:186810 1,4-Dihydropyridine derivatives for pharmaceutical compositions.
Materne, Carsten; Betzing, Hans (Nattermann, A., und Cie. G.m.b.H., Fed. Rep. Ger.). S. African ZA 7707702 **19780919**, 22 pp. (English).
CODEN: SFXXAB. APPLICATION: ZA 1977-7702 19771229.
GI

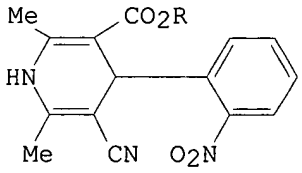


I

AB Dihydropyridinecarboxylates I (R = optionally substituted C3-12 alkyl) were prepd. for use as cerebral vasodilators. Thus, 2-O2NC6H4CHO was condensed with H2NCMe:CHCN and H2NCMe:CHCO2Pr to give 42% I (R = Pr). At 0.01-1 mg/kg i.v. in dogs I increase cerebral blood flow by 25-40%.
IC A61K031-44
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
IT 1694-31-1 5396-89-4 14205-46-0 **50899-08-6** 50899-10-0
53055-18-8 65482-22-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with nitrobenzaldehyde and aminocrotononitrile)
IT **50899-08-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with nitrobenzaldehyde and aminocrotononitrile)
RN 50899-08-6 HCA
CN Butanoic acid, 3-oxo-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)

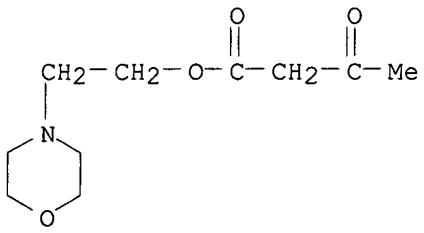


L9 ANSWER 25 OF 29 HCA COPYRIGHT 2003 ACS on STN
89:109135 1,4-Dihydropyridine derivatives. Materne, Carsten; Betzing, Hans (Nattermann, A., und Cie. G.m.b.H., Fed. Rep. Ger.). Ger. Offen. DE 2659665 **19780713**, 13 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 1976-2659665 19761230.
GI

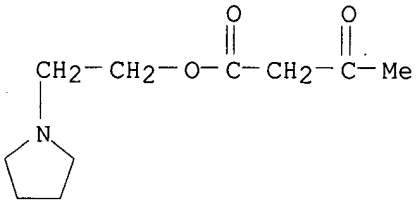


I

AB The phenylpyridines I (R = C1-12 alkyl optionally substituted by alkoxy, Ph, pyridyl, NH2, morpholine, etc.) were prepd. by the condensation of 2-O2NC6H4CHO(II), H2NCMe:CHCN (III), and MeCOCH2CO2R or H2NCMe:CHCO2R. Thus, a mixt. of II, H2NCMe:CHCO2Pr, III, EtOH, and HOAc was refluxed 1 h to give 42% I (R = Pr). I are useful as cerebral vasodilators, giving 25-40% in cerebral blood flow in dogs at 0.01-1 mg/kg i.v.
IC C07D211-90
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
IT 1694-31-1 5396-89-4 14205-46-0 **50899-08-6** 50899-10-0 53055-18-8 65482-22-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitrobenzaldehyde and aminocrotononitrile, cyano(nitrophenyl)nicotinate from)
IT **50899-08-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitrobenzaldehyde and aminocrotononitrile, cyano(nitrophenyl)nicotinate from)
RN 50899-08-6 HCA
CN Butanoic acid, 3-oxo-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 26 OF 29 HCA COPYRIGHT 2003 ACS on STN
82:170692 1,4-Dihydropyridine-3,5-dicarboxylic acid aminoalkyl ester derivatives. Iwanami, Masaru; Murakami, Masuo; Takahashi, Kozo; Fujimoto, Masaharu; Shibanuma, Tadao; Kawai, Ryutaro; Takenaka, Toichi (Yamanouchi Pharmaceutical Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 49109384 **19741017** Showa, 15 pp. (Japanese). CODEN: JKXXAF.
APPLICATION: JP 1973-25566 19730303.
GI For diagram(s), see printed CA Issue.
AB The pyridine derivs. I (R1 = alkyl; R2 = alkyl, ZNR3R4 (Z = alkylene; R3 = H, alkyl, aralkyl, aryl; R4 = alkyl, aralkyl, aryl; NR3R4 may form a heterocyclic ring); R5, R6 = H, halo, cyano, NO2, NH2, dialkylamino, CO2H, OH, alkoxy, SO3H, alkylsulfonyl, N3; X1 = O, S, CH:CH; R7 = alkyl; R8 = H, alkyl; R9 = alkyl, ZNR3R4] were prepd. by reaction of R1COCH2CO2R2 (II), III, and R7C(NHR8):CHCO2R9. I are vasodilating and hypotensive agents (no data). Thus, a mixt. of 3.9 g II (R1 = Me, R2 = Me2NCH2CH2), 1.7 g m-O2NC6H4CHO, 0.85 ml 28% NH4OH, and 5 ml EtOH was refluxed 5 hr to give 2.8 g bis[2-(dimethylaminoethyl) 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate. Among 24 more I similarly prepd. were Me (.beta.-dimethylaminoethyl) 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate, Et (.beta.-dimethylaminoethyl) 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate, Me (.beta.-pyrrolidinoethyl) 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate, and Me (1-methyl-2-dimethylaminoethyl) 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate.
NCL 16E431.1
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
IT 6131-49-3 **55985-43-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitrobenzaldehyde)
IT **55985-43-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitrobenzaldehyde)
RN 55985-43-8 HCA
CN Butanoic acid, 3-oxo-, 2-(1-pyrrolidinyl)ethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 27 OF 29 HCA COPYRIGHT 2003 ACS on STN
80:14958 Coronary dilating 1,4-dihydropyridine-3,5-dicarboxylates. Bossert, Friedrich; Meyer, Horst; Vater, Wulf (Bayer A.-G.). Ger. Offen. DE 2218644 **19731025**, 68 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 1972-2218644 19720418.
GI For diagram(s), see printed CA Issue.
AB Fifty-one dihydropyridines [I; R = H, Me, CHMe2, or Bu; R1 = Ph, substituted phenyl, (CH2)2Ph, CH:CHPh, 1-C10H7, 2-pyridyl, 2,6-dimethoxy-5-pyrimidinyl, 4-quinolyl, 2-bromo-5-furyl, or 2-nitro-5-thienyl; X = QR2 with Q = CHMeCH2 or (CH2)n, n = 1-3, and R2 = 2- or 3-pyridyl, morpholino, 4-methyl-1-piperazinyl, NMe2, or NEt2; Y = X or R3; R3 = Me, Et, CHMe2, or (CH2)2OMe] were prepd., mostly as hydrochlorides. I (X = Y) were prepd. by reaction of MeCOCH2CO2X (II) with R1CHO and RNH2. I (X = R3) were prepd. by reaction of II with R1CHO

and RNH-CMe:CHCO2R3 or with RNH2 and R1CH:C(COMe)CO2R3, or by reaction of I (X = H) with XCl. I had coronary dilating activity and were also useful e.g. as muscle relaxants and anti-hypertensives.

IC C07D

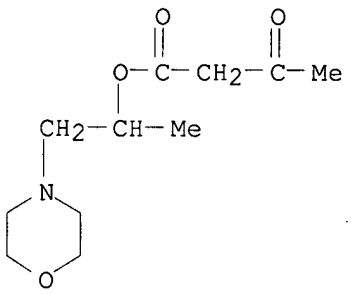
CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 27

IT 50899-05-3 50899-06-4 **50899-07-5 50899-08-6 50899-09-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with aldehydes and amino compds.)

IT **50899-07-5 50899-08-6 50899-09-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with aldehydes and amino compds.)

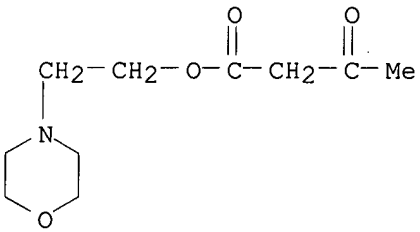
RN 50899-07-5 HCA

CN Butanoic acid, 3-oxo-, 1-methyl-2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)



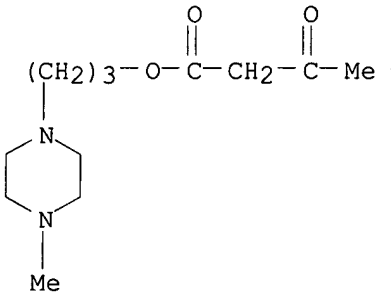
RN 50899-08-6 HCA

CN Butanoic acid, 3-oxo-, 2-(4-morpholinyl)ethyl ester (9CI) (CA INDEX NAME)

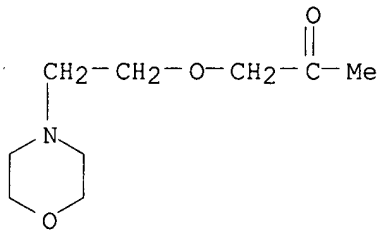


RN 50899-09-7 HCA

CN Butanoic acid, 3-oxo-, 3-(4-methyl-1-piperazinyl)propyl ester (9CI) (CA INDEX NAME)

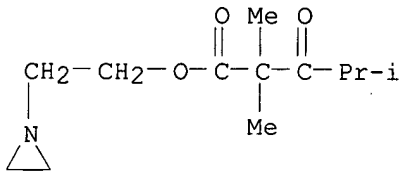


L9 ANSWER 28 OF 29 HCA COPYRIGHT 2003 ACS on STN
75:19654 Propargyl ether-oxides. Gautier, Jean A.; Miocque, Marcel; Moskowitz, Henri; Loisy, M. (Lab. Chim. Org., Fac. Pharm., Paris, Fr.). Annales Pharmaceutiques Francaises, 29(1), 39-56 (French) **1971**. CODEN: APFRAD. ISSN: 0003-4509.
AB The reactions of the triple bond and acetylenic H atom of ROCH2C.tplbond.CH (I) are studied. Thus, I are hydrogenated to give ROCH2CH:CH2 and hydrated to give ROCH2Ac. Aminobutynyl ethers, ROCH2C.tplbond.CCH2NMe2 are prepd. by the Mannich reaction. I are also alkylated, condensed with aldehydes, and converted into esters ROCH2C.tplbond.CCO2R1.
CC 23 (Aliphatic Compounds)
IT 929-70-4P 1746-13-0P 16488-93-0P 16488-95-2P 16488-96-3P
32827-36-4P 32833-36-6P 32833-37-7P 32833-38-8P 32833-39-9P
32833-41-3P 32833-42-4P 32833-43-5P 32833-44-6P 32833-45-7P
32833-46-8P 32833-47-9P 32833-48-0P 32833-49-1P
32833-50-4P 32833-51-5P 32833-52-6P 32833-53-7P 32833-54-8P
32833-55-9P 32833-56-0P 32833-57-1P 32833-58-2P 32833-59-3P
32833-60-6P 32833-61-7P 32833-62-8P 32833-63-9P 32833-64-0P
32833-65-1P 32833-66-2P 32833-67-3P 32833-69-5P 32833-70-8P
32833-71-9P 32833-72-0P 32978-41-9P 33064-48-1P 33302-46-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **32833-46-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 32833-46-8 HCA
CN 2-Propanone, 1-(2-morpholinoethoxy)- (8CI) (CA INDEX NAME)



L9 ANSWER 29 OF 29 HCA COPYRIGHT 2003 ACS on STN
68:49367 Reactions of 2,2,4,4-tetramethyl-1,3-cyclobutanedione with aziridines and other nucleophiles. Hansen, Gary Ralph; Burg, Tom E. (Univ. of Idaho, Moscow, ID, USA). Journal of Heterocyclic Chemistry, 4(4), 653-6 (English) **1967**. CODEN: JHTCAD. ISSN: 0022-152X.
GI For diagram(s), see printed CA Issue.
AB 2,2,4-Trimethyl-3-oxovaleric acid N-[2-(1-aziridinyl)ethyl]amide (I) and 2-(1-aziridinyl)ethyl 2,2,4-trimethyl-3-oxovalerate (II) are prepd. from the title ketone (III). III is treated with aziridine to give I, which is hydrolyzed to give ClCH2CH2NHCH2CH2NH2.2HCl. III is treated with N-(2-hydroxyethyl)aziridine to give II, which is refluxed with NaOH to give iso-Pr2CO. III is treated with N-butylaziridine and epoxyethylbenzene to give N,N'-dibutylpiperazine and iso-PrCO2CH2CH2Ph, resp.
CC 27 (Heterocyclic Compounds (One Hetero Atom))
IT 5590-29-4P 17330-28-8P **17330-29-9P** 17330-30-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **17330-29-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)
RN 17330-29-9 HCA
CN Valeric acid, 2,2,4-trimethyl-3-oxo-, 2-(1-aziridinyl)ethyl ester (8CI) (CA INDEX NAME)



Access DB# 101377

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sin J. Lee Examiner #: 76060 Date: 8-15-'0
Art Unit: 1752 Phone Number 30 5-0504 Serial Number: 09/ 994,808
Mail Box and Bldg/Room Location: 9B05 Results Format Preferred (circle) PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Amine Compounds, Resist compositions & Patterning Proc

Inventors (please provide full names): Hatakeyama, Jun; Kobayashi, Tomohiro; Watanabe, Takeru; Nagata, Takeshi

Earliest Priority Filing Date: 11-28-01

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for the amine compound of Claim. # 4

****

STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher:	NA Sequence (#)	STN
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#)	Questel/Orbit
Date Searcher Picked Up:	Bibliographic	Dr.Link
Date Completed:	Litigation	Lexis/Nexis
Searcher Prep & Review Time:	Fulltext	Sequence Systems
Clerical Prep Time:	Patent Family	WWW/Internet
Online Time:	Other	Other (specify)

PTO-1590 (8-01)

STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact ***the EIC searcher or contact*:**

Kathleen Fuller, EIC 1700 Team Leader
308-4290, CP3/4-3D62

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art **not found**:*
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC/EIC1700 CP3/4 3D62

=> file reg

****

Sin,

This printout corresponds to the structure in claim 4. If you have any additional questions please call me.

John

****

FILE 'REGISTRY' ENTERED AT 14:44:41 ON 04 SEP 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 SEP 2003 HIGHEST RN 577952-45-5
DICTIONARY FILE UPDATES: 2 SEP 2003 HIGHEST RN 577952-45-5

=> d his

(FILE 'HOME' ENTERED AT 14:08:05 ON 04 SEP 2003)

FILE 'REGISTRY' ENTERED AT 14:08:12 ON 04 SEP 2003
ACTIVATE LEE808/A

L1 STR
L2 SCR 1608 AND 1838 AND 1210 AND 1707
L3 SCR 1839 OR 2016 OR 2026 OR 1918 OR 1929 OR 2043 OR 1267 OR 170
L4 1038 SEA FILE=REGISTRY SSS FUL L1 AND L2 NOT L3

FILE 'LREGISTRY' ENTERED AT 14:08:31 ON 04 SEP 2003
L5 STR L1

FILE 'REGISTRY' ENTERED AT 14:11:27 ON 04 SEP 2003
L6 3 S L5 SSS SAM SUB=L4

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FILE 'REGISTRY' ENTERED AT 14:13:12 ON 04 SEP 2003
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SAVE L7 LEE808II/A

FILE 'HCA' ENTERED AT 14:13:53 ON 04 SEP 2003
L8 29 S L7

FILE 'REGISTRY' ENTERED AT 14:14:30 ON 04 SEP 2003

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     FILE 'HCA' ENTERED AT 14:15:27 ON 04 SEP 2003
L9           29 S L8 AND 1907-2001/PY,PRY
L10      102802 S RESIST## OR PHOTORESIST? OR PHOTOLITH?
L11           0 S L9 AND L10

     FILE 'LREGISTRY' ENTERED AT 14:17:32 ON 04 SEP 2003
L12             STR L1

     FILE 'REGISTRY' ENTERED AT 14:25:33 ON 04 SEP 2003
L13          12 S L12 SSS SAM  SUB=L4
L14             STR L12
L15          11 S L14 SSS SAM  SUB=L4
L16             STR L14
L17           8 S L16 SSS SAM  SUB=L4
L18         161 S L16 SSS FULL  SUB=L4
                SAVE L18 LEE808STR4/A
L19         130 S L18 AND 1-25/C

     FILE 'LREGISTRY' ENTERED AT 14:32:59 ON 04 SEP 2003

     FILE 'HCA' ENTERED AT 14:33:41 ON 04 SEP 2003
L20          93 S L19
L21          91 S L20 AND 1907-2000/PY,PRY

     FILE 'LREGISTRY' ENTERED AT 14:34:35 ON 04 SEP 2003
L22             STR L18

     FILE 'REGISTRY' ENTERED AT 14:36:17 ON 04 SEP 2003
L23           3 S L22 SSS SAM  SUB=L4
L24           3 S L22 SSS SAM  SUB=L4
L25         110 S L22 SSS FULL  SUB=L4
L26          77 S L25 AND 1-20/C

     FILE 'HCA' ENTERED AT 14:38:24 ON 04 SEP 2003
L27          65 S L26
L28          64 S L27 AND 1907-2000/PY,PRY
L29           1 S L28 AND L10
L30          27 S L21 NOT L27
L31          29 S L9 NOT L29
L32          63 S L28 NOT L29
L33          27 S L30 NOT L29

     FILE 'REGISTRY' ENTERED AT 14:43:27 ON 04 SEP 2003

     FILE 'HCA' ENTERED AT 14:43:58 ON 04 SEP 2003

     FILE 'REGISTRY' ENTERED AT 14:44:41 ON 04 SEP 2003

=> d que stat L18
L1              STR
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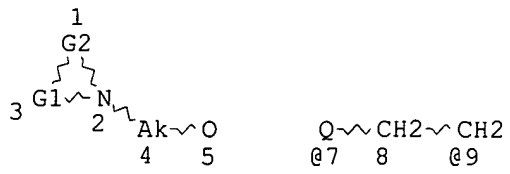


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REP G1=(1-4) CH2
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REP G2=(0-5) 7-3 9-2
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CONNECT IS E2  RC AT   5
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT   4
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
L2              SCR 1608 AND 1838 AND 1210 AND 1707
L3              SCR 1839 OR 2016 OR 2026 OR 1918 OR 1929 OR 2043 OR 1267 O
R 1700 OR 1304
L4         1038 SEA FILE=REGISTRY SSS FUL L1 AND L2 NOT L3
L16             STR
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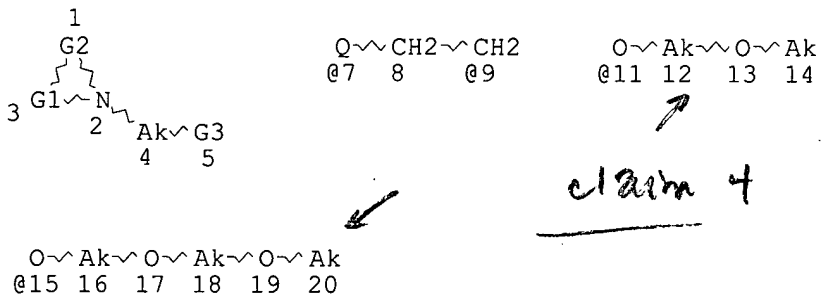

claim 4

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REP G1=(1-4) CH2
REP G2=(0-5) 7-3 9-2
VAR G3=OH/11/15
NODE ATTRIBUTES:
CONNECT IS E3  RC AT   2
CONNECT IS E2  RC AT   4
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT   4
GGCAT   IS SAT  AT  12
GGCAT   IS SAT  AT  14
GGCAT   IS SAT  AT  16
GGCAT   IS SAT  AT  18
GGCAT   IS SAT  AT  20
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE
L18          161 SEA FILE=REGISTRY SUB=L4 SSS FUL L16

100.0% PROCESSED   1038 ITERATIONS                    161 ANSWERS
SEARCH TIME: 00.00.01


=> file hca
FILE 'HCA' ENTERED AT 14:45:11 ON 04 SEP 2003
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FILE COVERS 1907 - 28 Aug 2003 VOL 139 ISS 10
FILE LAST UPDATED: 28 Aug 2003 (20030828/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

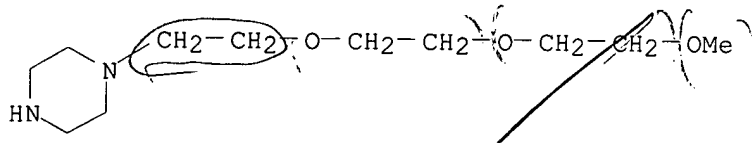
=> d L32 1,3,7,9,12,14,16,19,21,27,30,34,36,39,40,41,43,47,50-51,52,54,56,59,61,63 cbib abs hitstr

L32 ANSWER 1 OF 63 HCA COPYRIGHT 2003 ACS on STN
136:200481 Preparation of water-soluble thiazolyl peptide derivatives. Naidu, B. Narasimhulu; Li, Wenying; Lam, Kin S.; Sorenson, Margaret E.; Wichtowski, John A.; Connolly, Timothy P.; Ueda, Yasutsugu; Bronson, Joanne J.; Zhang, Yunhui; Kim, Oak K. (Bristol-Myers Squibb Company, USA). PCT Int. Appl. WO 2002014354 A1 20020221, 90 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US25560 20010815. PRIORITY: US 2000-PV225598 20000815.

AB Novel thiazolyl peptides R1-Y-CH2CH(Q)CONH2 [Q is a residue of a thiazolyl peptide antibiotic, e.g., nocathiacin I or nosiheptide; Y = S, SO, SO2 or NR, where R = H, OH, alkoxy, alkanoyl, alkylcarbamoyl, etc.; R1 = 1-azabicyclo[2.2.2]oct-3-yl or N-oxide, [(CH2)2O]1-3(CH2)2R4' (R4' = OH, amino, phenylmethyl), or (un)substituted alkyl] were prepd. for use in pharmaceutical compns. for the treatment of serious bacterial infections. Thus, a peptide prepd. by Michael addn. reaction of nocathiacin I with 1-methylpiperazine showed in vitro antibiotic activity 0.25, 0.125, and 0.5 .mu.g/mL (MIC) against Staphylococcus aureus, Streptococcus pneumoniae, and Enterococcus faecalis, resp.

IT **400836-58-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of water-sol. thiazolyl peptide derivs.)

RN 400836-58-0 HCA
CN Piperazine, 1-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



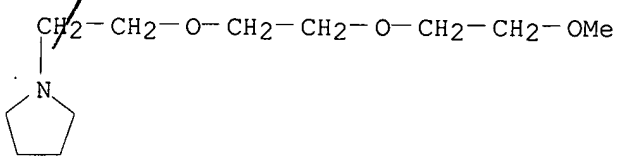
L32 ANSWER 3 OF 63 HCA COPYRIGHT 2003 ACS on STN
133:147416 Antimycobacterial activity of ionic fullerene derivatives. Bosi, Susanna; Da Ros, Tatiana; Castellano, Sabrina; Banfi, Elena; Prato, Maurizio (Dipartimento di Scienze Farmaceutiche, Universita di Trieste, Piazzale Europa 1, Trieste, 34127, Italy). Bioorganic & Medicinal Chemistry Letters, 10(10), 1043-1045 (English) **2000**. CODEN: BMCLE8. ISSN: 0960-894X. Publisher: Elsevier Science Ltd..

AB Pos. charged fullerene derivs., moderately sol. in water:DMSO 9:1, have been tested using three strains of Mycobacterium spp. Some compds. inhibit the growth of Mycobacterium tuberculosis, a human clin. isolate, particularly virulent and resistant, at doses as low as 5 .mu.g/mL.

IT **287402-41-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(antimycobacterial activity of pyrrolidines)

RN 287402-41-9 HCA

CN Pyrrolidine, 1-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 7 OF 63 HCA COPYRIGHT 2003 ACS on STN
124:261768 Urea-containing hydroxyethylamine peptides as retroviral protease inhibitors. Talley, John J.; Getman, Daniel P.; Freskos, John N.; Lin, Ko-chung; Heintz, Robert M.; Rogier, Jr Donald J.; Bertenshaw, Deborah E. (Monsanto Co., USA). U.S. US 5475013 A **19951212**, 60 pp.
Cont.-in-part of U.S. Ser. No. 789,642, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1992-886531 19920520. PRIORITY: US 1990-615210 19901119; US 1991-789642 19911220.

GI

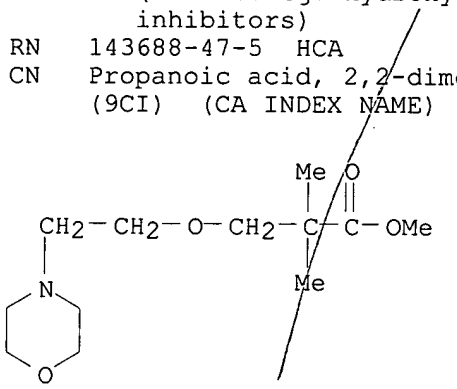
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Urea-contg. peptide compds. I or their pharmaceutically acceptable salts, prodrugs, or esters thereof, wherein: A = radical represented by the formulas II, RR'N(CR1'R1'')qCHR1C(:Y'), III; R = e.g., H, alkoxycarbonyl, aralkoxycarbonyl; R' = e.g., H and radicals as defined for R3; q = 0, 1; R1 = e.g., H, CH2SO2NH2, CO2Me, amino acid side chains; R1', R1'' = e.g., H and radicals defined for R1; R2 = e.g., alkyl, aryl, cycloalkyl; R3 = e.g., alkyl, alkenyl, alkynyl; X' = e.g., O, CR17 where R17 = H, alkyl, and N; Y, Y', Y'' = O, S, NR15 wherein R15 = H and radicals as defined for R3; B = CR7R7'(CH2)nR8; n = 0-6; R7 and R7' = e.g., radicals as defined

for R3 and amino acid side chains; R8 = e.g., CN, OH, alkyl, alkoxy; R4 = H and radicals defined by R3; R6 = H, alkyl; R20, R21, R30, R31, R32 = e.g., radicals as defined for R1; R33, R34 = e.g., H, radicals as defined for R3; are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease. Thus, e.g., Curtius rearrangement of 2,2-dimethyl-3-(4-pyridyl)propionic (prepn. given) with diphenylphosphoryl azide, followed by coupling with 3(S)-[N-(2-quinolinylcarbonyl)-L-asparaginyl]amino-2(R)-hydroxy-4-phenylbutyl-N-(4-fluorophenylmethyl)amine afforded butanediamide, N1-[3-[[[(1,1-dimethyl-2-(4-pyridyl)ethyl)amino]carbonyl](4-fluorophenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, [1S-[1R*(R*),2S*]] (IV) which inhibited HIV protease with IC50 = 4 nM.

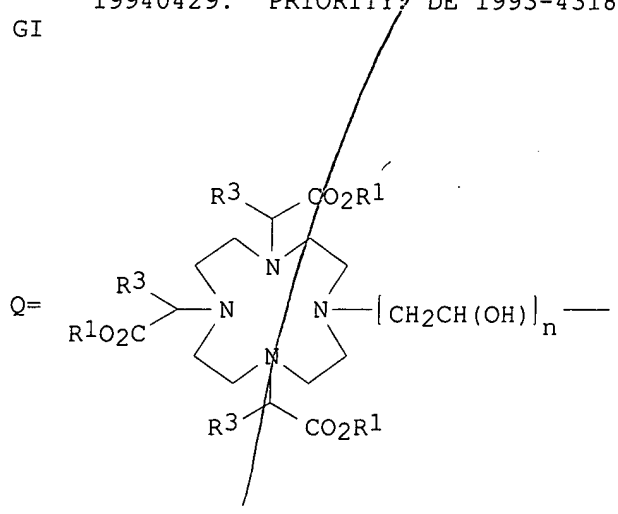
IT **143688-47-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(urea-contg. hydroxyethylamine peptides as retroviral protease inhibitors)

RN 143688-47-5 HCA
CN Propanoic acid, 2,2-dimethyl-3-[2-(4-morpholinyl)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



L32 ANSWER 9 OF 63 HCA COPYRIGHT 2003 ACS on STN
123:228230 Preparation of N,N,N-tricarboxymethyl-1,4,7-10-tetraazacyclododecane metal complexes as NMR diagnostic temperature probes. Platzek, Johannes; Raduechel, Bernd; Niedballa, Ulrich; Weinmann, Hanns-Joachim; Bauer, Hans; Roth, Klaus (Schering A.-G., Germany). PCT Int. Appl. WO 9427977 A1 **19941208**, 56 pp. DESIGNATED STATES: W: CA, JP, NO, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (German). CODEN: PIXXD2. APPLICATION: WO 1994-EP1376 19940429. PRIORITY: DE 1993-4318369 19930528.

GI



AB RZA [R = tetraazacyclododecyl(hydroxyethyl) group Q; A = H or Q; R1 = H,

metal ion; R3 = H, (un)substituted alkyl; Z = (O- or CO-interrupted) (un)substituted alkylene; n = 0 or 1] were prepd. Thus, QH (R1 = R3 = H, n = 0) was N-alkylated by MeOCH2CH2Br to give QCH2CH2OMe (R1 = R3 = H, n = 0) which was stirred 5h at 85.degree. with Pr2O3 in water to give the Pr complex. The latter was administered i.v. to rats and variation of chem. shift with body temp. data were given.

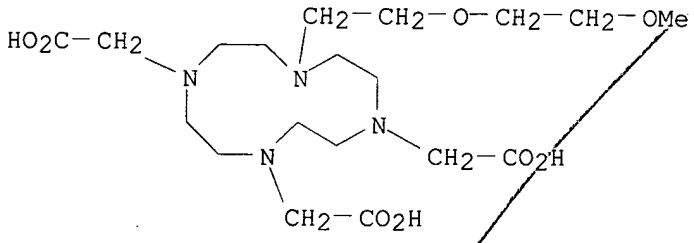
IT **168078-37-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of N,N,N-tricarboxymethyl-1,4,7-10-tetraazacyclododecane metal complexes as NMR diagnostic temp. probes)

RN 168078-37-3 HCA

CN 1,4,7,10-Tetraazacyclododecane-1,4,7-triacetic acid, 10-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 12 OF 63 HCA COPYRIGHT 2003 ACS on STN

122:182777 Single ring crown ether and .beta.-galactosidase for sodium ion determination. Umemoto, Atsushi; Tadano, Toshio (Kyowa Medex Co Ltd, Japan). Jpn. Kokai Tokkyo Koho JP 06217797 A2 **19940809** Heisei, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1993-11924 19930127.

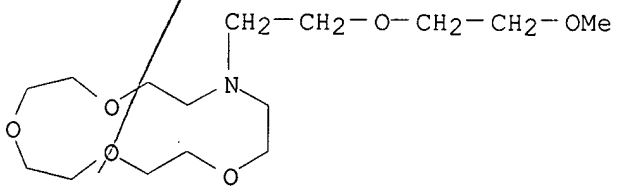
AB Disclosed is a method for Na+ detn. by measuring the reaction of .beta.-galactosidase and its substrate in the presence of a single ring crown ether. In example, 18-crown-6 or N-[2-(methoxyethoxy)ether]monoazo-15-crown-5 were used to prep. std. curves for Na+ detn.

IT **79402-96-3**

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (single ring crown ether and .beta.-galactosidase for sodium ion detn.)

RN 79402-96-3 HCA

CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 14 OF 63 HCA COPYRIGHT 2003 ACS on STN

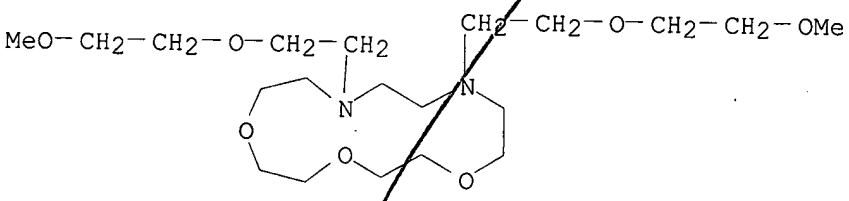
120:174803 Thermodynamics of Macrocycle Complexation Chemistry. Interactions of Metal Ions with Double-Armed N-Pivot Lariat Ethers in Methanol and Methanol-Water Solutions at 25.0 .degree.C. Izatt, Reed M.; Zhang, Xianxin; An, Haoyun; Zhu, Cheng Y.; Bradshaw, Jerald S. (Department of Chemistry, Brigham Young University, Provo, UT, 84602, USA). Inorganic Chemistry, 33(6), 1007-10 (English) **1994**. CODEN: INOCAJ. ISSN: 0020-1669.

AB Log K, .DELTA.H, and T.DELTA.S values for interactions of Na+, K+, Cu2+, and Ca2+ with a series of N,N'-dipivot lariat ethers have been detd. from calorimetric titrn. data valid in 9:1 (vol./vol.) CH3OH/H2O and abs. methanol at 25.0 .degree.C. Complex stability is increased greatly by introducing pendant arms contg. oxygen or nitrogen atoms to the parent macrocycles. The enthalpy and entropy changes support the idea that the side arms interact with the cations. Formation of complexes of Ca2+ is both enthalpy and entropy stabilized. All other interactions are enthalpy driven, and the entropy changes are unfavorable. Effects of pendant-arm length and substituents on the complexation of the cations are discussed on the basis of the thermodn. data. The large neg. .DELTA.H values for complexation of Cu2+ with lariat ethers indicate a strong interaction between Cu2+ and the nitrogen atoms of the ligands. Large entropic losses for some of the cation-ligand interactions indicate that the lariat ethers are flexible and readily change their conformations to accommodate the cations.

IT **134540-86-6D**, metal complexes
RL: PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(stability const. and thermodn. of formation of)

RN 134540-86-6 HCA

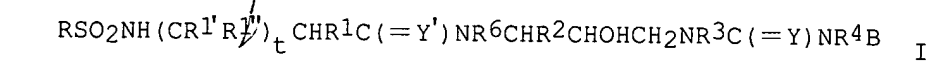
CN 1,4,7-Trioxa-10,13-diazacyclopentadecane, 10,13-bis[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 16 OF 63 HCA COPYRIGHT 2003 ACS on STN

118:234479 Preparation of sulfonylaminoamides as HIV protease inhibitors. Reed, Kathryn Lea; Talley, John Jeffrey (Monsanto Co., USA). PCT Int. Appl. WO 9208699 A1 **19920529**, 175 pp. DESIGNATED STATES: W: AU, CA, CS, FI, HU, JP, KR, NO, PL, SU; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1991-US8593 19911118. PRIORITY: US 1990-615210 19901119; US 1991-789645 19911114.

GI



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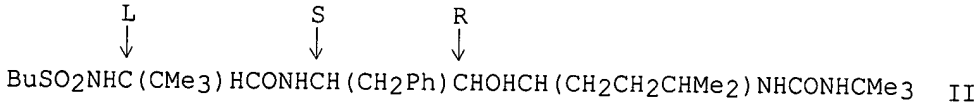


II

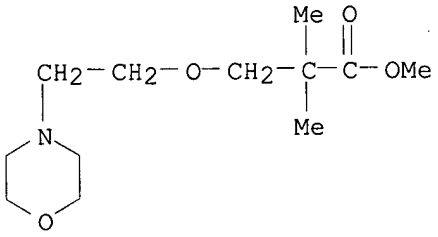
AB Title compds. I [R = (hydroxy)alkyl, alkenyl, cycloalkyl(alkyl), heterocycloalkyl, aryl, (hetero)aralkyl; t = 0, 1; R1 = CH2SO2NH2, (cyclo)alkyl, amino acid side chains selected from asparagine, glycine, leucine, phenylalanine, alanine, etc.; R1', R1'' = H, groups defined for R1; R2 = (cyclo)alkyl, aryl, etc.; R3 = (hydroxy)alkyl, alkenyl, cycloalkyl(alkyl), heterocycloalkyl, aryl, etc.; Y, Y' = O, S; B = R5,

CR7R7'(CH2)nR8; R4, R5 = groups defined for R3; NR4R5 = heterocycloalkyl, heteroaryl; R6 = H, groups defined for R3; n = 0-6; R7, R7' = groups defined for R3, amino acid side chains selected from valine, isoleucine, glycine, alanine, asparagine, etc.; CR7R7' = cycloalkyl; R8 = cyano, OH, alkoxy, (cyclo)alkyl, etc.] were prepd. as HIV protease inhibitors useful for the treatment of AIDS. Thus, N-(n-butylsulfonyl)-L-tert-butylglycine was coupled with (2R,3R)-3-amino-1-isoamyl-1-(tert-butylcarbamoyl)amino-4-phenyl-2-butanol in the presence of hydroxybenzotriazole and Me2N(CH2)3N:C:NEt.HCl in DMF to give title compd. II. I had IC50 of 22-24 nM against HIV protease.

IT **143688-47-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for HIV protease inhibitors)

RN 143688-47-5 HCA

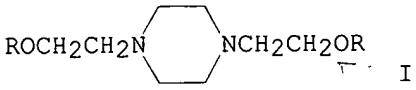
CN Propanoic acid, 2,2-dimethyl-3-[2-(4-morpholinyl)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



L32 ANSWER 19 OF 63 HCA COPYRIGHT 2003 ACS on STN

116:255637 Catalytic processes for the preparation of bridged nitrogen-containing compounds. King, Stephen Wayne (Union Carbide Chemicals and Plastics Co., Inc., USA). Eur. Pat. Appl. EP 476780 A2 **19920325**, 16 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1991-202423 19910919. PRIORITY: US 1990-585565 19900920.

GI

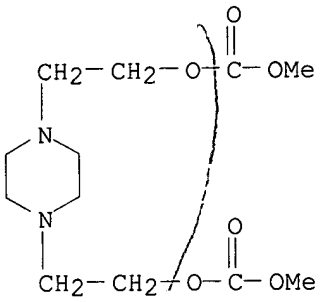


AB Bridged N compds. were prepd. by contg. a carboxylated cyclic N compd. with a mixed metal oxide catalyst. Thus, diol. I (R = H) was treated with (MeO)2CO to give ester I (R = CO2Me) which was treated at 350.degree. in MeOCH2CHMeOMe with a MgO-Al2O3 catalyst to give 33.4% triethylenediamine.

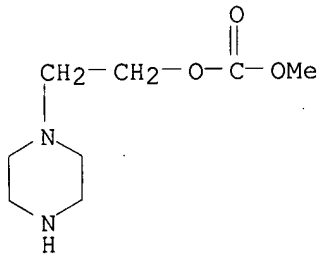
IT **141578-01-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and decarboxylation of, catalyst for)

RN 141578-01-0 HCA

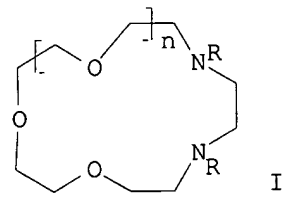
CN Carbonic acid, 1,4-piperazinediyldi-2,1-ethanediyl dimethyl ester (9CI) (CA INDEX NAME)



IT **141578-00-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 141578-00-9 HCA
CN Carbonic acid, methyl 2-(1-piperazinyl)ethyl ester (9CI) (CA INDEX NAME)



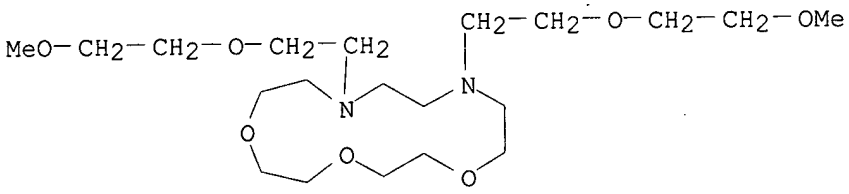
L32 ANSWER 21 OF 63 HCA COPYRIGHT 2003 ACS on STN
115:49656 Preparation of N,N'-di pivot lariat 1,4-diaza-15-crown-5 and 18-crown-6 macrocycles. An, Haoyun; Bradshaw, Jerald S.; Izaat, Reed M. (Dep. Chem., Brigham Young Univ., Provo, UT, 84602, USA). Journal of Heterocyclic Chemistry, 28(2), 469-72 (English) **1991**. CODEN: JHTCAD. ISSN: 0022-152X. OTHER SOURCES: CASREACT 115:49656.
GI



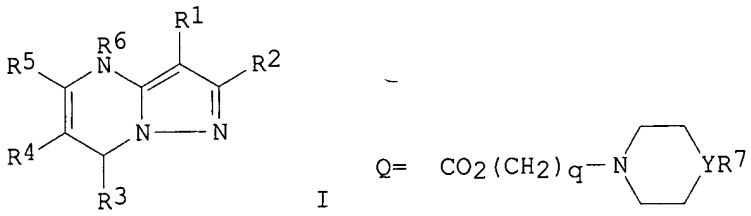
I

AB Twelve diaza-15-crown-5 and 18-crown-6 macrocycles, e.g. I (R = CH2CH2OCH2CH2OMe, n = 1, 2), contg. different side arms on the nitrogen atoms have been prepd. These diaza-N,N'-di pivot lariat crown ethers were prepd. either from N,N'-bishydroxyethyl-1,4-diaza-15-crown-5 or 18-crown-6 ligands or from the corresponding unsubstituted diaza-crowns. Thus, I (R = CH2CH2OCH2CH2OMe, n = 1) was prepd. by condensing I (R = CH2CH2OH, n = 1) (II) with TsOCH2CH2OMe (Ts = 4-MeC6H4SO2) in THF. II was prepd. by the cyclocondensation of HOCH2CH2NHCH2CH2NHCH2CH2OH with TsOCH2(CH2OCH2)3CH2OTs.

IT **134540-86-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 134540-86-6 HCA
CN 1,4,7-Trioxa-10,13-diazacyclopentadecane, 10,13-bis[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



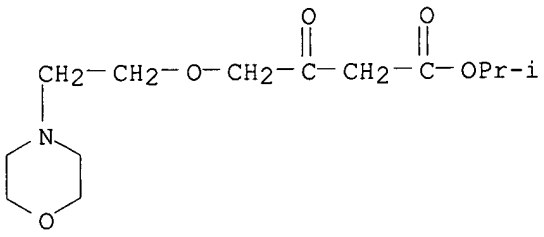
L32 ANSWER 27 OF 63 HCA COPYRIGHT 2003 ACS on STN
109:149558 Preparation of 4,7-dihydropyrazolo[1,5-a]pyrimidine derivatives as calcium antagonists. (Yoshitomi Pharmaceutical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 63060985 A2 **19880317** Showa, 39 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1987-198872 19870807. PRIORITY: CA 1986-515584 19860808.
GI



AB The title compds. [I; R1 = CHO, PhCO, C1-8 alkanoyl; R2 = H, halo, NO2, NH2, acylamino, C1-8 alkyl, C3-8 cycloalkyl, cyano, CO2H, CONH2, CHO, etc.; R3 = H, C1-8 alkyl, C2-10 alkenyl, C2-10 alkynyl, (un)substituted aryl, (un)substituted Ph, etc.; R4 = H, NO2, cyano, acyl, (mono- or disubstituted) CONH2 or C(S)NH2, (unsubstituted CO2H; R5 = H, cyano, C1-8 alkyl, haloalkyl, hydroxyalkyl, aminoalkyl, CHO, NH2, (un)substituted Ph or aralkyl, etc.; R6 = H, C1-8 alkyl, haloalkyl, hydroxyalkyl, aminoalkyl, acyl, heteroaryl, (un)substituted aralkyl], having Ca antagonist or Ca agonist/antagonist activities (no data) and useful as, e.g. antihypertensives, were prepd. A soln. of 3.0 4-[2-(phthalimido)ethoxy]-3-oxobutyric acid iso-Pr ester (II) (prepn. given) and 1.5 g 2,3-F2C6H3CHO in benzene contg. 2 drops each of AcOH and piperidine was refluxed for 3 h with removal of H2O by a Dean-Stark trap. After removing the solvent, 1.1 g 3-amino-4-cyanopyrazole and 10 mL DMF was added to the residue and the mixt. was heated at 100.degree. for 6 h to give 1.65 g I [R1 = cyano, R2 = R6 = H, R3 = 2,3-F2C6H3, R4 = CO2CHMe2, R5 = 2-(phthalimido)ethoxy] which was treated with H2NNH2.H2O in MeOH-CHCl3 at 50.degree. for 5 h to give, after conversion into a HCl salt, I (R5 = H2NCH2CH2O, R1-R4,R6 as defined above).HCl.

IT **116646-24-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with benzaldehyde deriv.)
RN 116646-24-3 HCA

CN Butanoic acid, 4-[2-(4-morpholinyl)ethoxy]-3-oxo-, 1-methylethyl ester (9CI) (CA INDEX NAME)

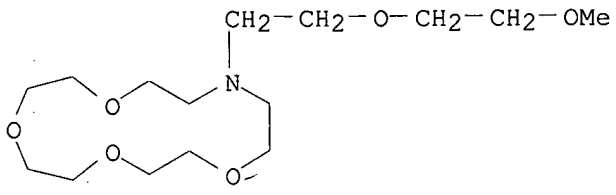


L32 ANSWER 30 OF 63 HCA COPYRIGHT 2003 ACS on STN
107:28880 Mechanism of complexation of sodium(1+) with N-pivot-lariat 15-crown-5 ethers in methanol at 25.degree.C. Echegoyen, Luis; Gokel, George W.; Kim, Min Sook; Eyring, Edward M.; Petrucci, Sergio (Dep. Chem., Univ. Miami, Coral Gables, FL, 33124, USA). Journal of Physical Chemistry, 91(14), 3854-62 (English) **1987**. CODEN: JPCHAX. ISSN: 0022-3654.

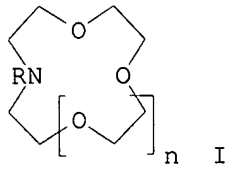
AB Ultrasonic relaxation absorption spectra were detd. for 0.1-0.3M NaClO4 + 0.1-0.3M methoxyethoxyethylmonazo 15-crown-5 ether (RN15C5) in MeOH at 25.degree. and 0.5-400 MHz. The data are interpreted by the 2-step scheme: Na+ + RN15C5 .dblarw. Na+, RN15C5 .dblarw. (Na+RN15C5), where the intermediate represents a complex species with Na+ residing outside the crown ether ring. The role of the side chain was also studied by ultrasonic relaxation techniques with the crown ether monoazomethyl 15C5 (MeN15C5) (having only a -CH3 appendage) + NaClO4 in MeOH. Two concn.-dependent, Debye relaxation processes were obsd. with this crown ether. This suggests that the role of the side chain is only marginal in detg. the presence of the upper frequency relaxation process. An isomeric single Debye process whose relaxation frequency is independent of concn. is obsd. for both crown ethers dissolved in MeOH (at comparable frequencies with those reported) when Na+ is also present. 15C5 contg. only C and O atoms in the ring shows no relaxation process in MeOH at comparable concns. and 25.degree.. This suggests that the upper relaxation process is assocd. with the inversion of the lone electron pair of the N (rather than with the rearrangement of the side chain.). A mol. analogy between RN15C5 crown ether and 221 cryptand is drawn. As a further test of the supposition that the upper relaxation of both RN15C5 and MeN15C5 when reacting with Na+ is due to N inversion, the isomeric relaxation of 221 cryptand in MeOH was studied. Two Debye relaxations appear, probably assocd. with the inversions of both the nitrogens of 221 cryptands, in analogy with a previous interpretation of the ultrasonic relaxation of 222 cryptand in water by Schneider et al. (1981). With Na+ reacting with 221, a double Debye relaxation also appears, consistent with the above hypothesis. The role of the side chain of RN15C5, when compared with MeN15C5 reacting with Na+ in MeOH, appears mainly to be that of enhancing the stability of the final complex, with Na+ embedded in the cavity of the crown ether possibly coordinated also to the side chain. The influence of the cation on the 2 relaxations obsd. in MeOH solns. of NH4ClO4 plus MeN15C5 is also reported. Surprisingly, AgClO4 + MeN15C5 shows only a single relaxation at a frequency comparable to that attributes to the isomeric process, although the relaxation amplitude (max. excess sound absorption per wavelength) is different from that of the isomeric process.

IT **79402-96-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation by, of sodium in methanol, ultrasonic relaxation study

of)
RN 79402-96-3 HCA
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 34 OF 63 HCA COPYRIGHT 2003 ACS on STN
103:178252 12-, 15-, and 18-Membered-ring nitrogen-pivot lariat ethers: syntheses, properties, and sodium and ammonium cation binding properties. Schultz, Rose Ann; White, Banita D.; Dishong, Dennis M.; Arnold, Kristin A.; Gokel, George W. (Dep. Chem., Univ. Miami, Coral Gables, FL, 33124, USA). Journal of the American Chemical Society, 107(23), 6659-68 (English) **1985**. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 103:178252.
GI

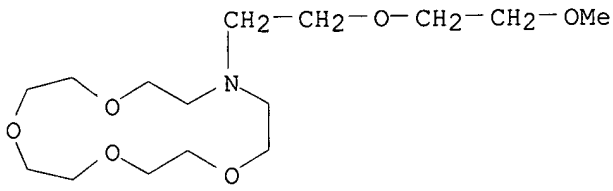


AB N-pivot lariat ethers of varying ring sizes can be prepd. by cyclization of an amine or substituted diol. 12-Membered ethers I [R = PhCH2, 2-, 4-MeOC6H4, 2-MeOC6H4CH2, HO(CH2)3, Me2NCH2CH2, MeOCH2CH2; n = 1] were prepd. by the method of M. Calverley and J. Dale (1982); this involves cyclo-bis-dialkylation of an amine with 1,11-diiodo-3,6,9-trioxaundecane. I (R = 2-O2NC6H4CH2, 3,6-dioxaheptyl, 3,6,9-trioxadecyl, 3,6,9,12-tetraoxatridecyl, 11-allyloxy-3,6,9-trioxaundecyl; n = 1) did not form in high yield by this method or were more conveniently prepd. by alkylation of I (R = H, n = 1). The latter was prepd. from I (R = PhCH2, n = 1) by hydrogenolysis. Monoaza-15-crown-5 derivs. I (R = allyl, Bu, Me3C, PhCH2, MeOCH2CH2, 3,6-dioxaheptyl, 3,6,9,12,15,18,21,24-octaoxapentacosyl, 2-MeOC6H4, 4-MeOC6H4, 2-MeOC6H4CH2; n = 2) were prepd. by cyclizing RN(CH2CH2OH)2 with R1(OCH2CH2)3OR1 (R1 = MeSO2, 4-MeC6H4SO2). I (R = Me, 2-O2NC6H4CH2, 4-O2NC6H4CH2, Me3CO2CCH2, n =2) were prepd. by the alkylation of I (R = H, n = 2) which was prepd. by hydrogenolysis I (R = PhCH2, n = 2). Monoaza-18-crown-6 derivs. I (R = H, Me, PhCH2, MeOCH2CH2, 3,6-dioxaheptyl, 3,6,9-trioxadecyl, 3,6,9,12-tetraoxatridecyl, 3,6,9,12,15-pentaoxahexadecyl, 3,6,9,12,15,18,21,24-octaoxapentacosyl, 2-MeOC6H4; n = 3) were analogously prepd. Studies involving NH4 cation binding show that the interaction of ring and side-chain with the cation is intramol. in MeOH soln.; the Na cation binds similarly. X-ray crystal structure evidence confirms this for the solid state in the I (R = 2-MeOCH2CH2, n = 3).cntdot.KI complex. The strongest binding for Na occurs when 6 O are present, regardless of ring size, which suggests that a flexible macrocycle is directed by the cation to envelop and solvate in

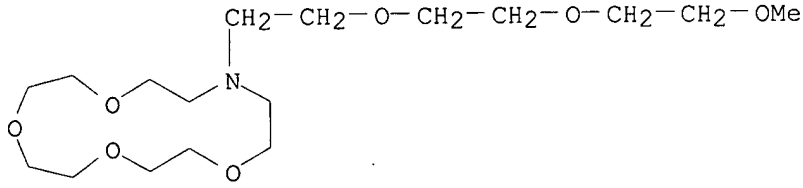
the geometry most appropriate for the cation.

IT **79402-96-3P 80755-60-8P 80755-63-1P 80755-64-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and binding consts. of, for ammonium and sodium cations)

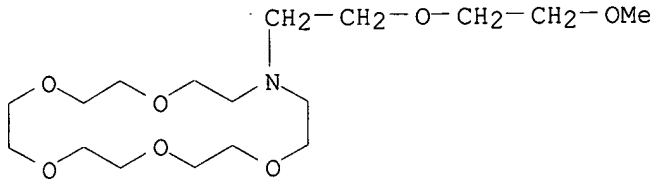
RN 79402-96-3 HCA
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



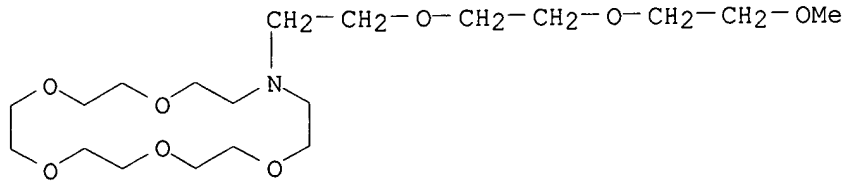
RN 80755-60-8 HCA
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 80755-63-1 HCA
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



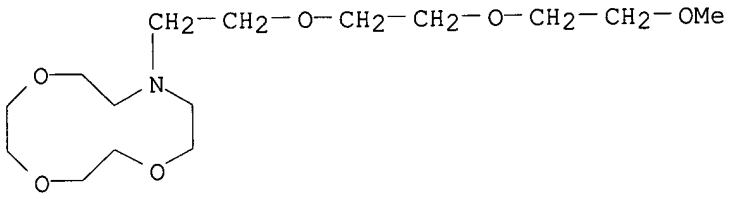
RN 80755-64-2 HCA
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



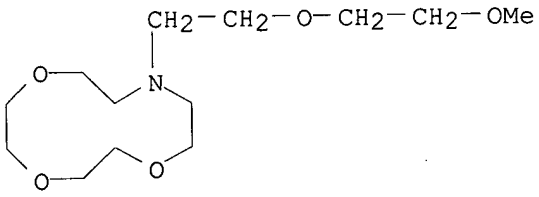
IT **96530-20-0P 98269-19-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 96530-20-0 HCA
CN 1,4,7-Trioxa-10-azacyclododecane, 10-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]-

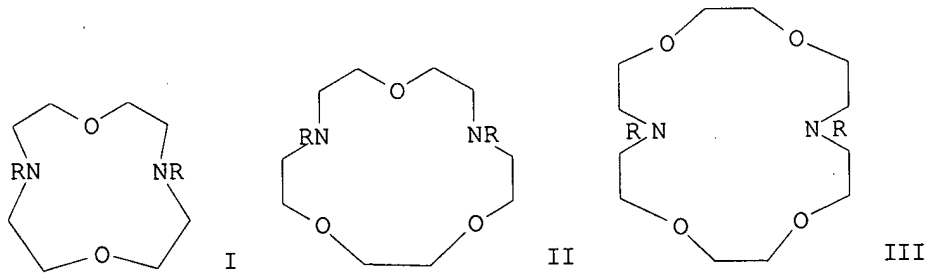
(9CI) (CA INDEX NAME)



RN 98269-19-3 HCA
CN 1,4,7-Trioxa-10-azacyclododecane, 10-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)

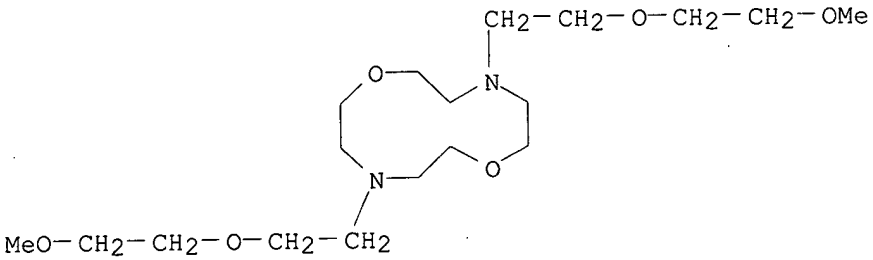


L32 ANSWER 36 OF 63 HCA COPYRIGHT 2003 ACS on STN
102:220328 Mass spectra of a new type of crown ethers. Fu, Guixiang; Wu, Yuanwei; Xu, Xiaoyun; Lu, Huixiung; Cheng, Dekai; Sheng, Huaiyu (Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China). Huaxue Xuebao, 43(2), 150-4 (Chinese) **1985**. CODEN: HHHPA4. ISSN: 0567-7351.
GI

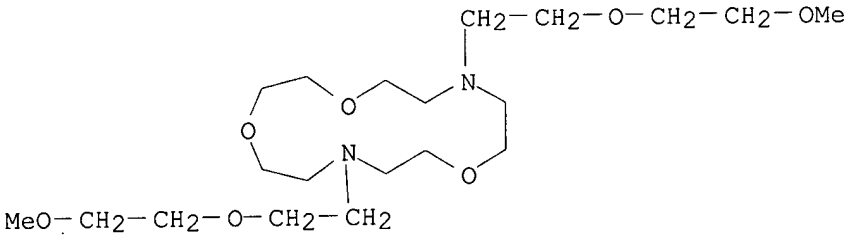


I II III

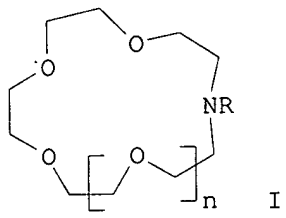
AB The electron-ionization mass spectra of crown ethers [I, II, III; R = MeO(CH2)2, BuO(CH2)2O(CH2)2, MeO(CH2)2O(CH2)2O(CH2)2, etc.] were studied. The fragmentation pathways were discussed with the aid of metastable anal.
IT **85726-94-9 87057-97-4**
RL: PRP (Properties)
(electron-ionization mass spectra of)
RN 85726-94-9 HCA
CN 1,7-Dioxa-4,10-diazacyclododecane, 4,10-bis[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



RN 87057-97-4 HCA
CN 1,4,10-Trioxa-7,13-diazacyclopentadecane, 7,13-bis[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)

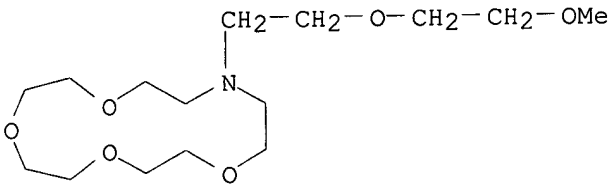


L32 ANSWER 39 OF 63 HCA COPYRIGHT 2003 ACS on STN
101:90992 Nitrogen-containing polyether macrocycles with a sidearm containing neutral electron donor groups. Gokel, George W. (Grace, W. R., and Co., USA). U.S. US 4436664 A **19840313**, 8 pp. Cont.-in-part of U.S. Ser. No. 203,165, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1982-339530 19820115. PRIORITY: US 1980-198981 19801021; US 1980-203165 19801103.
GI

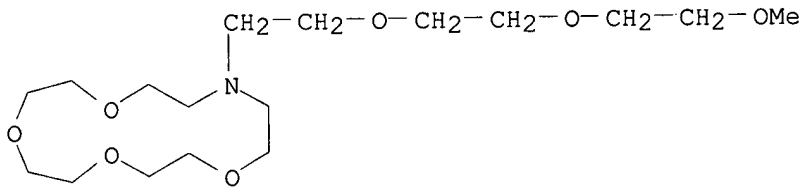


AB Title macrocycles I [R = 2-(alkoxy)malkyl, 2-alkoxyphenyl, 2-alkoxyphenylmethyl, 2-alkoxyphenylethyl, aminoalkyl, 2-aminophenyl; n = 0, 1, 2; m = 1, 4] were prepd. as cation binding agents and phase-transfer catalysts. Thus, MeSO3(CH2CH2O)4SO2Me was cyclized with CHOCH2CH2)2NCH2CH2OMe to give 53% I (R = MeOCH2CH2, n = 2) (II). The binding K values of II for Na+ in MeOH was 38,019.
IT **79402-96-3P 80755-60-8P 80755-63-1P 80755-64-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and binding of, with sodium ion)

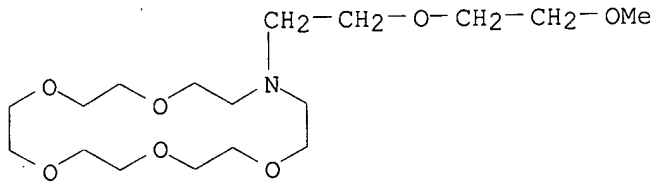
RN 79402-96-3 HCA
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



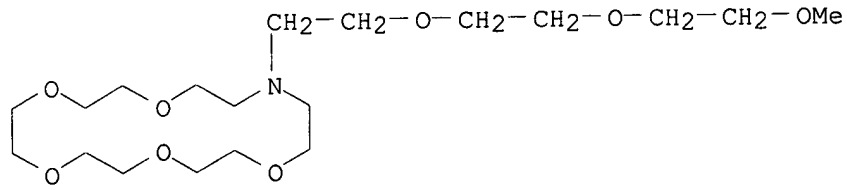
RN 80755-60-8 HCA
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



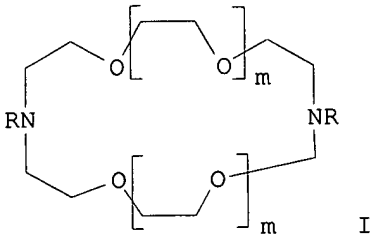
RN 80755-63-1 HCA
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



RN 80755-64-2 HCA
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 40 OF 63 HCA COPYRIGHT 2003 ACS on STN
100:209771 Synthesis and coordination properties of new macrocyclic polyethers. Sheng, Huaiyu; Li, Shusen; Lu, Huixiu; Cheng, Dekai (Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China). Huaxue Xuebao, 41(12), 1127-36 (Chinese) **1983**. CODEN: HHHPA4. ISSN: 0567-7351. OTHER SOURCES: CASREACT 100:209771.
GI



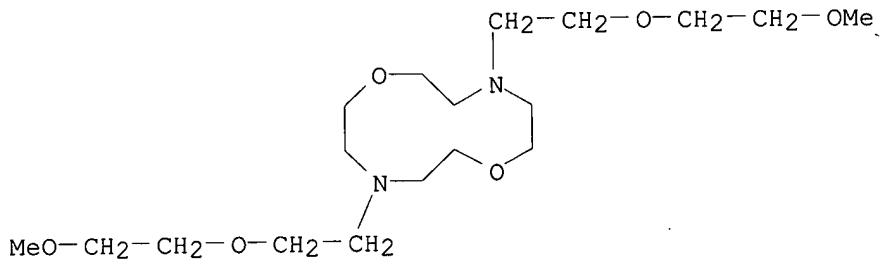
I

AB Polyethers I [m = 0, 1; R = Q (Q = CH2(CH2OCH2)nCH2OR1, R1 = Me, Bu); n = 0-2](II) were prepd. in 30-65% yields by reaction of I (R = H) with BrQ. II complexed readily with alkali cations with high selectivity for Na+ and K+.

IT **85726-94-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coordination properties of)

RN 85726-94-9 HCA

CN 1,7-Dioxa-4,10-diazacyclododecane, 4,10-bis[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 41 OF 63 HCA COPYRIGHT 2003 ACS on STN

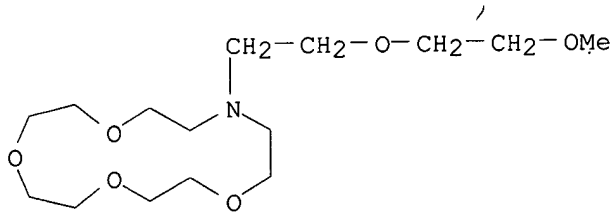
100:74856 Sodium(1+) complexation with new multidentate polyether ligands - rapid estimation of complex stabilities by sodium-23 NMR spectroscopy. Offermann, Werner; Weber, Edwin (Fachbereich Chem. Biol., Univ. Bremen, Bremen, D-2800/33, Fed. Rep. Ger.). Chemische Berichte, 117(1), 234-45 (German) **1984**. CODEN: CHBEAM. ISSN: 0009-2940.

AB A new 23Na NMR method for fast and simple estn. of Na+ complex stabilities is reported and applied to various polyether ligands. Synthesis of new coronands and podands are described.

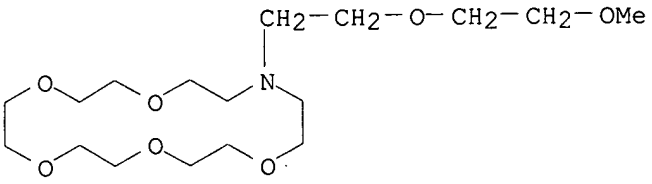
IT **79402-96-3P 80755-63-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(NMR and prepn. of)

RN 79402-96-3 HCA

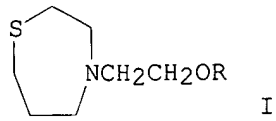
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



RN 80755-63-1 HCA
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)

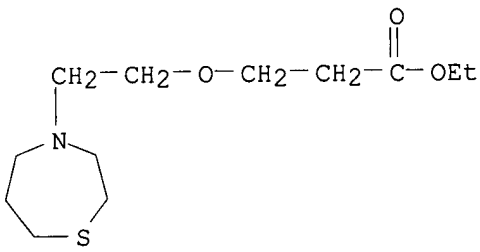


L32 ANSWER 43 OF 63 HCA COPYRIGHT 2003 ACS on STN
99:5608 Perhydro-1,4-thiazepine derivatives with expected pharmacological activity. Part II. 2-(Perhydro-1,4-thiazepin-4-yl)ethyl benzyl and benzhydryl ethers with mycostatic and anthelmintic activity. Strzelczyk, Marek (Dep. Gen. Chem. Physiol. Biochem., Military Med. Acad., Lodz, 90-647, Pol.). Polish Journal of Pharmacology and Pharmacy, Volume Date 1982, 34(4), 265-73 (English) **1983**. CODEN: PJPPAA. ISSN: 0301-0244. OTHER SOURCES: CASREACT 99:5608.
GI



I

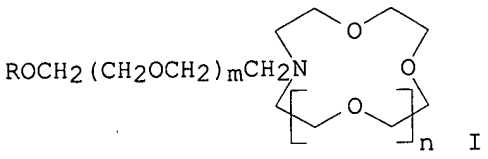
AB Title ethers I [R = PhCH2, PhOCH2CH2, 2,4-Cl2C6H3CH2, 2-BrC6H4CH2, Ph2CH, 4-ClC6H4CHPh, EtO2CCH2CH2] were prepd. by etherification of 4-(2-hydroxy- or 2-chloroethyl)perhydro-1,4-thiazepine. I (R = PhOCH2CH2 or 2-BrC6H4CH2) showed the highest mycostatic and anthelmintic activities. Spectral data are given.
IT **86010-81-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra, and anthelmintic activities of)
RN 86010-81-3 HCA
CN Propanoic acid, 3-[2-(tetrahydro-1,4-thiazepin-4(5H)-yl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)



L32 ANSWER 47 OF 63 HCA COPYRIGHT 2003 ACS on STN
96:199651 Complexing ability of N-oligoethylene glycol monoaza crown ethers with sodium and potassium cations. Masuyama, Araki; Nakatsuji, Yohji; Ikeda, Isao; Okahara, Mitsuo (Dep. Appl. Chem., Osaka Univ., Osaka, 565, Japan). Tetrahedron Letters, 22(46), 4665-8 (English) **1981**.

CODEN: TELEAY. ISSN: 0040-4039.

GI



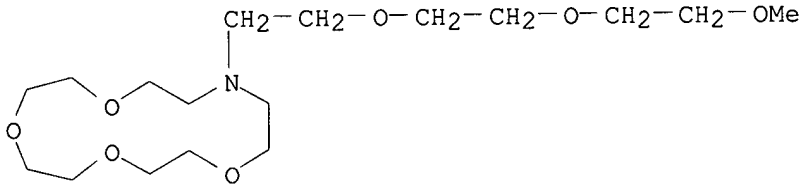
I

AB The monoaza crown ethers I (n = 2, 3; m = 0-2, R = H; m = 2, R = Me) were prepd. and the stability consts. of their Na+ and K+ complexes were detd. For the 18-crown-6 derivs. the max. stability was obtained with 1 and 2 oxyethylene units, resp., in the side chain for Na+ and K+, whereas for the 15-crown-5 derivs., 1-unit-longer oxyethylene chains were necessary for max. cation-complexing ability. The complexing abilities are optimum when the cation fits the cavity formed by the monoaza crown ring and the oligoethylene glycol side chain.

IT **80755-60-8P 80755-64-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and complexation of, with sodium and potassium cations)

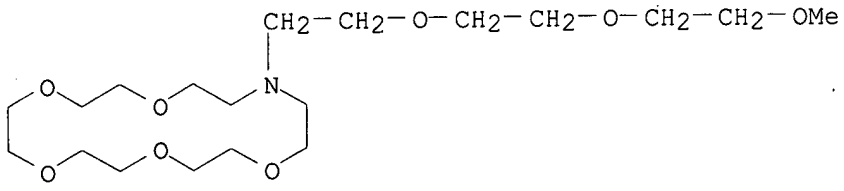
RN 80755-60-8 HCA

CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 80755-64-2 HCA

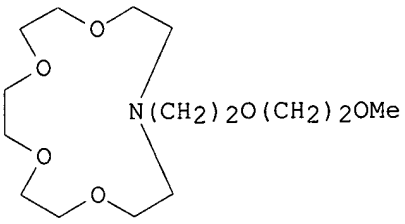
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 50 OF 63 HCA COPYRIGHT 2003 ACS on STN

95:169154 Crown-cation complex effects. 14. Lariat ethers. 3. Macrocyclic polyethers bearing donor groups on flexible arms attached at a nitrogen pivot point. Schultz, Rose Ann; Dishong, Dennis M.; Gokel, George W. (Dep. Chem., Univ. Maryland, College Park, MD, 20742, USA). Tetrahedron Letters, 22(28), 2623-6 (English) **1981**. CODEN: TELEAY. ISSN: 0040-4039.

GI



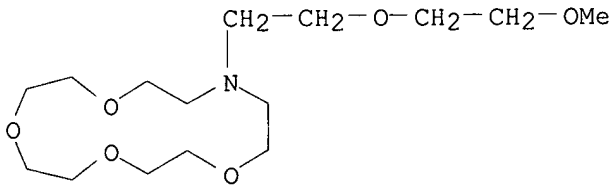
I

AB Eight lariat ethers with a N pivot atom for the donor sidearm (e.g., I) were prepd. by reaction of N-alkylated ethanolamines with triethylene glycol di-p-toluenesulfonate (NaH, THF) and their Na+ binding consts. were measured. In some cases, the binding is enhanced considerably relative to C-based ethers. This effect may be due to diminished "sidedness".

IT **79402-96-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and complexation of, with sodium cation)

RN 79402-96-3 HCA

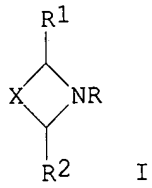
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 51 OF 63 HCA COPYRIGHT 2003 ACS on STN

95:132649 Cycloamine derivatives and their use as tertiary heterocyclic amines as synergists in pesticides. Himmelreich, Rolf G.; Spiess, Wolfram (Spiess, C. F., und Sohn G.m.b.H. und Co. Chemische Fabrik, Fed. Rep. Ger.). Eur. Pat. Appl. EP 29617 **19810603**, 25 pp. (German). CODEN: EPXXDW. APPLICATION: EP 1980-200923 19801001.

GI

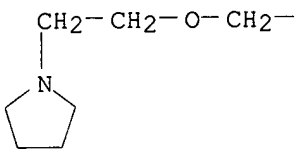


I

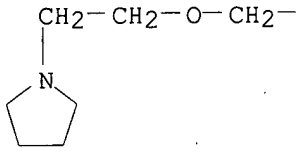
AB The cyclic amines I (R = optionally substituted aliph. group; R1, R2 = H, Me, Et; X = CH2OCH2, (CH2)n; n = 0-5] were prepd. as synergists for insecticides, e.g., pyrethroids, phosphates, or carbamates (test data tabulated). Thus, Br(CH2)10Me reacted with hexamethylenimine in CH2Cl2 to give I [R = undecyl, R1 = R2 = H, X = (CH2)4].

IT **79089-26-2 79089-38-6 79089-64-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(insecticide synergist activity of)

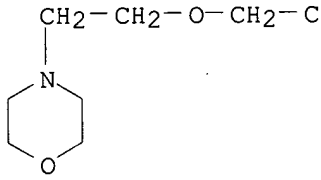
RN 79089-26-2 HCA
CN Pyrrolidine, 1-[2-[2-(2-butoxyethoxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 79089-38-6 HCA
CN Pyrrolidine, 1-[2-(2-butoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



RN 79089-64-8 HCA
CN Morpholine, 4-[2-(2-butoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)

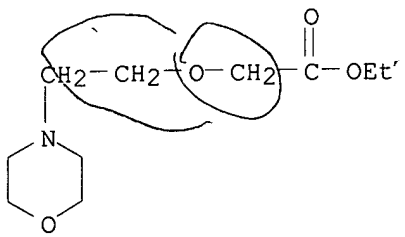


L32 ANSWER 52 OF 63 HCA COPYRIGHT 2003 ACS on STN
95:80179 Oxaalkanoate antiulcer composition. Laughlin, Robert G.; Fu, Juian-Juian L. (Procter and Gamble Co., USA). U.S. US 4263281 **19810421**, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1979-57922 19790716.

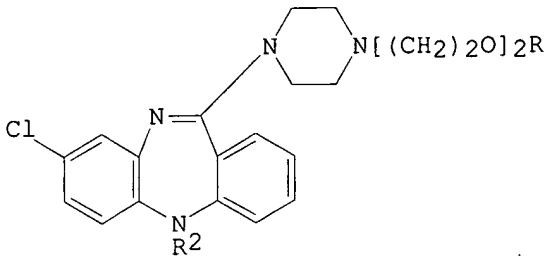
AB Zwitterionic compds. R3N+ZCO2- (at least one R group is a lipophilic hydrocarbyl group contg. >10 C atoms and the remainder are hydrocarbyl contg. <10 C atoms; Z = oxyalkylene with a chain length of .ltoreq.11 total atoms), useful in the prevention or treatment of ulcers, were prepd. Thus, Me2NCH2CH2OCH2CH2CN was converted to Me(CH2)21N+Me2CH2CH2OCH2CH2CO2- via Me2NCH2CH2OCH2CH2CO2Et and Me(CH2)21N+Me2CH2CH2OCH2CH2CO2Et Br-.

IT **78546-50-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and quaternization of)

RN 78546-50-6 HCA
CN Acetic acid, [2-(4-morpholinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

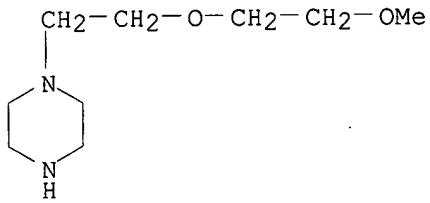


L32 ANSWER 54 OF 63 HCA COPYRIGHT 2003 ACS on STN
94:15779 8-Chloro-11-(4-substituted-1-piperazinyl)5H-dibenzo[b,e][1,4]diazepines and their use in pharmaceutical compositions. (Abbott Laboratories, USA). Brit. GB 1562874 **19800319**, 9 pp. (English). CODEN: BRXXAA. APPLICATION: GB 1978-7097 19780222.
GI

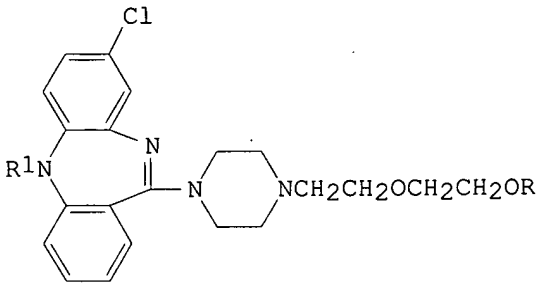


I

AB The title compds. I [R = H, alkyl, hydroxyalkyl, COR1 (R1 = C1-15 alkyl); R2 = H, COR1], useful as antischizophrenics, were prepd. E.g., 8-chloro-10,11-dihydro-11-oxo-5H-dibenzo[b,e][1,4]diazepine on sequential chlorination with PCl5 and condensation reaction with (1-hydroxyethoxyethyl)piperazine gave I (R = R2 = H). The activities of I were assessed in rats. Compns. contg. I are described.
IT **68465-66-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with dichlorodibenzodiazepine)
RN 68465-66-7 HCA
CN Piperazine, 1-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 56 OF 63 HCA COPYRIGHT 2003 ACS on STN
90:6429 Dibenzo[b,e][1,4]diazepines. Horrom, Bruce Wayne; Minard, Frederick Nelson; Zaugg, Harold Elmer (Abbott Laboratories, USA). Ger. Offen. DE 2807568 **19780831**, 24 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 1978-2807568 19780222.
GI



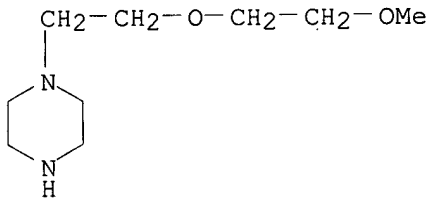
I

AB Dibenzodiazepines I (R = H, lower alkyl, hydroxyalkyl, C2-15 acyl; R1 = H, C2-15 acyl) were prepd. Thus, 8-chloro-10,11-dihydro-11-oxo-5H-dibenzo[b,e][1,4]-diazepine was treated with PCl5 and the imino chloride treated with 1-[2-(2-hydroxyethoxy)ethyl]piperazine to give I (R = R1 = H). Rats treated with 0.15 mmol I (R = R1 = H)/kg i.p. had 2.8 times the homovanillic acid level in the brain of controls.

IT **68465-66-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichlorodibenzodiazepine)

RN 68465-66-7 HCA

CN Piperazine, 1-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 59 OF 63 HCA COPYRIGHT 2003 ACS on STN

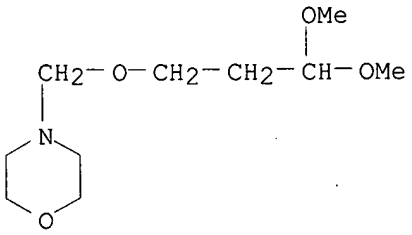
71:40136 Preparation of easily dyeable poly(vinyl alcohol) synthetic fibers with a low degree of discoloration. Uzumaki, Mitsutaka; Takashio, Masahiko; Shirosaka, Akihisa (Japan Vinyl Co., Ltd.). Jpn. Tokkyo Koho JP 43019115 B4 **19680819** Showa, 3 pp. (Japanese). CODEN: JAXXAD. APPLICATION: JP 19651016.

AB Poly(vinyl alc.) (10% aq.) 100, H2SO4 10, 3-morpholinopro-pionaldehyde di-Me acetal 1.8, and water 1.8 parts, were heated 5 hrs. at 60.degree.. 3-Morpholinopropionacetalized poly(vinyl alc.) thus prepd. was mixed with poly(vinyl alc.), and poly(vinyl alc.) mixts. contg. 0.06, 0.12, 0.18, and 0.24% N were prepd., and 8% spinning solns. were prepd. from these mixts. The pH's of these solns. were adjusted to give films having a low degree of discoloration during heat treatment. Heat-treated films thus prepd. showed high dye affinity toward direct dyes, and the acetylated films with an aq. soln. of 20% sulfuric acid and 5% formic acid were not affected by boiling water.

IT **24899-99-8**
RL: USES (Uses)
(reaction products, with poly(vinyl alc.), vinal fibers contg., dyeable nondiscoloring on heating)

RN 24899-99-8 HCA

CN Propionaldehyde, 3-(morpholinomethoxy)-, dimethyl acetal (8CI) (CA INDEX NAME)



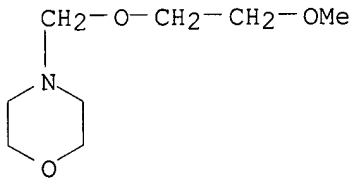
L32 ANSWER 61 OF 63 HCA COPYRIGHT 2003 ACS on STN
60:3147 Original Reference No. 60:518h,519a-b Reactions of 2-naphthol with N-piperidinomethyl and N-mor- pholinomethyl alkyl ethers. Fernandez, J. E.; Powell, Charles; Fowler, Joanna S. (Univ. of South Florida, Tampa). Journal of Chemical and Engineering Data, 8(4), 600 (Unavailable) **1963**. CODEN: JCEAAX. ISSN: 0021-9568.

AB .alpha.-Amino ethers of the general formula RR'NCH2OR'', where RR'N is a morpholino or piperidino group and R'' is an alkyl, alkenyl, or alkynyl group, are prepd. according to McLeod and Robinson (CA 15, 3977). The following .alpha.-amino ethers (product, d2525, n25D, pKa, and b.p. given) are prepd.: 1-ethoxymethylpiperidine, -, -, 9.63, b1 52-8.degree.; 1-[(2-methoxyethoxy)methyl]piperidine, 0.9539, 1.4514, 9.75, b16 76-7; 1-(allyloxymethyl)piperidine, 0.9150, 1.4567, 9.60, b11 79-80.degree.; 1-(propargyloxymethyl)piperidine, 0.9899, 1.4723, 9.50, b12 82.5-3.degree.; N-(ethoxymethyl)morpholine, -, -, 7.38, b1 55-6.degree.; N-[(2-methoxyethoxy)methyl]morpholine, 1.0415, 1.4501, 7.43, b36 111-13.degree.; N-(allyloxymethyl)morpholine, -, -, 7.29, b8 80.degree.; N-(propargyloxymethyl)morpholine, 1.0476, 1.4698, 6.95, b1 65-8.degree.. The pKa values are detd. from the half-neutralization point of the titration curve. The prepd. ethers are treated with 2-C10H7OH to give 1-piperidinomethyl-2-hydroxynaphthalene and 1-morpholinomethyl-2-hydroxynaphthalene.

IT **90867-89-3**, Morpholine, 4-[(2-methoxyethoxy)methyl]- (prepn. of)

RN 90867-89-3 HCA

CN Morpholine, 4-[(2-methoxyethoxy)methyl]- (7CI) (CA INDEX NAME)



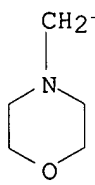
L32 ANSWER 63 OF 63 HCA COPYRIGHT 2003 ACS on STN
34:41208 Original Reference No. 34:6287e-i,6288a-d Solid derivatives of monoalkyl ethers of ethylene glycol and diethylene glycol. Mason, J. Philip; Manning, Joseph F. Journal of the American Chemical Society, 62, 1635-40 (Unavailable) **1940**. CODEN: JACSAT. ISSN: 0002-7863.

AB Since the ordinary derivs. of alcs. were not solids when cellosolves and carbitols are used, it is necessary to introduce some other group into the mol. and then make a solid deriv. by means of a reaction involving the new group. .beta.-Methoxyethoxyacetic acid and the EtO analog (Palomaa and Siitonen, C. A. 25, 2417)yield p-phenylphenacyl esters m. 68.degree. (61.5% yield) and 52.5-2.8.degree. (51.5% yield). The formation of these esters is rather slow. Because of the low m. p. and yield, the method was not applied to other derivs. Piperazonium di-.beta.-ethoxyethoxyacetate,

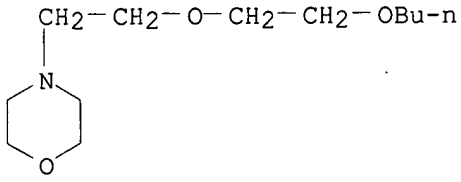
m. 87-7.5.degree. (85.6%); MeO analog, m. 44.5-5.degree. (79%); there is a tendency for these derivs. to sep. as oils or gummy solids. p-Nitrobenzoates were prepd. by the method of Conn, Collett and Lazzell (C. A. 27, 61) and that of Adams (C. A. 20, 2322); the b. ps. at 16 mm. and yields by Adams method are: MeOC2H4OH (I) 192.5-5.degree., 81.3%; EtOC2H4OH (II) 197-9.degree., 73.6%; BuOC2H4OH (III) 208.8-11.degree., 82%; EtOC2H4OC2H4OH (IV) 222.5-4.degree., 68.3%; BuOC2H4OC2H4OH (V) 246-9.degree., 77.3%. These may be reduced by Fe and HCl but better results are obtained with Sn and HCl. p-Aminobenzoates: I b16 217.5-9.degree., m. 79.7.degree., 68%; II b16 223-4.5.degree., m. 79.2.degree., 83.3%; III b16.5 232.5-4.degree., m. 36.2-6.5.degree., 80.8%; IV, b20 257-9.degree., m. 64.4.degree., 59.7%; V b16 262.5-5.degree., 81.8% (IV and V are new). p-(.beta.-Alkoxycarbethoxy)- and p-[.beta.-(.beta.'-alkoxyethoxycarbethoxy)]benzeneazo-p'-dimethylanilines were prepd. in the usual way through the diazo reaction: I, m. 108.2.degree., 88.5%; II m. 103.degree., 90%; III m., 73.8.degree., 81.6%; IV m. 87.8-8.4.degree., 72.8%; V m. 57.2.degree., 78.6%. Since the prepn. of these compds. involves esterification, reduction, diazotization and coupling, it is hardly satisfactory from the standpoint of qual. analysis. Reduction of the p-nitrobenzoate of II with Zn and NH4Cl gives a mixt. of products from which the p-aminobenzoate and p,p'-di(.beta.-ethoxycarbethoxy)azobenzene were isolated. The Na derivs. of I-V and .beta.-4-morpholinoethyl chloride (VI) (cf. preceding abstr.), refluxed 45 min., give the .beta.-4-morpholinoethyl esters, which were characterized by the picrates (prepd. in aq. or alc. soln.) and the HCl salts; b. ps. and yields of the esters and the m. ps. of the 2 derivs. are given: I b8 119-20.degree., 71.6%, 111.3.degree., 97.2-7.5.degree.; II b10 132-3.degree., 69.7%, 111.1.degree., 99.5-100.5.degree.; III b9 154-7.degree., 66.5%, 62-2.5.degree., 59.5-60.degree.; IV b9 163-5.degree., 60.5%, 204.8-7.degree., 150-1.degree.; V b8 189-92.degree., 58%, 161-1.5.degree., -. A typical procedure for identifying these compds. is as follows: 2 g. II in 6 cc. dioxane and 0.23 g. Na are refluxed until the reaction is complete; 1.4 g. of VI is then added and the mixt. refluxed for 1 hr.; after cooling 15 cc. 30% NaOH is added, the ether layer removed, washed twice with 10% NaOH and then heated on the steam bath for 15-20 min. to remove the last traces of solvent; aq. picric acid is added until the mixt. remains turbid and then 4 cc. excess and the mixt. kept in the refrigerator for 2-3 hrs.; the yield is 54.3%. The total time before the crystn. is about 2.5 hrs., of which 2 hrs. are used for refluxing and evapn. II (38.2 g.), 15 g. (HCHO)x and 37 g. Et2NH give 46.5% of diethylaminomethyl .beta.-ethoxyethyl ether, b16 73-4.5.degree.; it yields a gummy picrate, decomps. with dry HCl but appears to yield an ethiodide, m. 164.degree..

IT **76092-00-7**, Morpholine, 4-[2-(2-methoxyethoxy)ethyl]-
79089-64-8, Morpholine, 4-[2-(2-butoxyethoxy)ethyl]-
(and salts)

RN 76092-00-7 HCA
CN Morpholine, 4-[2-(2-methoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



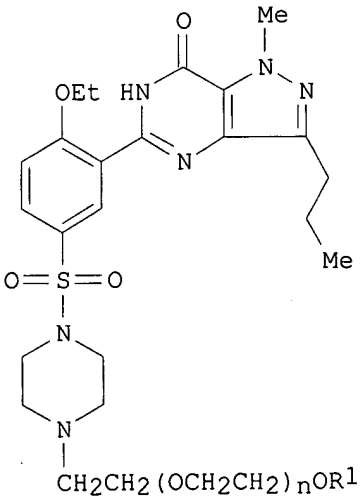
RN 79089-64-8 HCA
CN Morpholine, 4-[2-(2-butoxyethoxy)ethyl]- (9CI) (CA INDEX NAME)



=> d L30 1,5,10,15,20,25-27 cbib abs hitstr

L30 ANSWER 1 OF 27 HCA COPYRIGHT 2003 ACS on STN
136:210608 Preparation of polyethoxylated pyrazolo-pyrimidinone derivatives and their pharmaceutical compositions for the treatment of impotence. Chung, Bong-Youl; Lee, In-Sang; Park, Bong-Jun; Kim, Young-Keun; Kim, Sung-Ji; Yoon, Seung-Hyun (LG Chem Investment Ltd., S. Korea). PCT Int. Appl. WO 2002016364 A1 20020228, 37 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-KR951 20000823.

GI



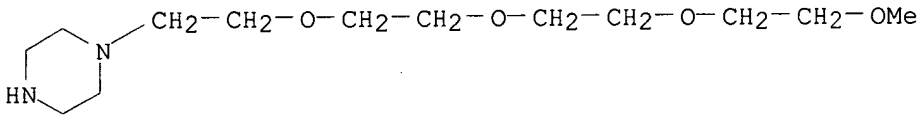
I

AB The present invention relates to polyethoxylated pyrazolopyrimidinone derivs. (I; R1 = H, alkyl, cycloalkyl, perfluoroalkyl, alkenyl, alkynyl, alkoxyalkyl; n = 2-400) or pharmaceutically acceptable salts thereof, process for prepn. thereof and pharmaceutical compns. comprising the same for the treatment of impotence and other diseases, such as angina, hypertension, congestive heart failure and atherosclerosis. In addn., the present invention relates to intermediates produced during the above process and the process for prepn. thereof. For example, 5

polyethoxylated pyrazolo-pyrimidinone derivs. were prepd. The soly. of the compds. is about 20-200 times higher than that of sildenafil citrate (Viagra). The compds. showed a high relaxation rate for corpus cavernosum penis in rabbits;. They had 10 times higher reaction threshold concn. and exhibit 4-5 times more excellent relaxation effect at the same concn. of 10-4M, when compared with sildenafil citrate.

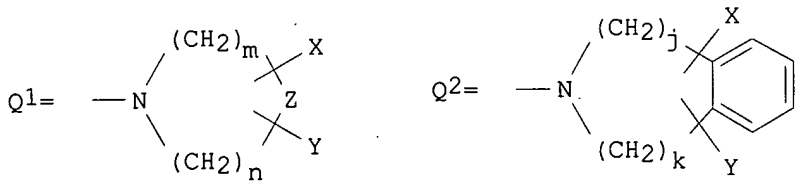
IT **400836-57-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of polyethoxylated pyrazolo-pyrimidinone derivs. and their pharmaceutical compns. for the treatment of impotence and cardiovascular disorders)

RN 400836-57-9 HCA
CN Piperazine, 1-(3,6,9,12-tetraoxatridec-1-yl)- (9CI) (CA INDEX NAME)



L30 ANSWER 5 OF 27 HCA COPYRIGHT 2003 ACS on STN
126:19324 Preparation of arylsulfonylamino acid amide trypsin and thrombin inhibitors.. Hoyle, William; Howarth, Graham Arton; Brundish, Derek Edward; Kane, Peter Daniel; Walker, Clive Victor; Hayler, Judy; Fullerton, Joseph David; Smith, Garric Paul; Wathey, William Bernard; et al. (Ciba-Geigy A.-G., Switz.). PCT Int. Appl. WO 9629327 A1 **19960926**, 202 pp. DESIGNATED STATES: W: AL, AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-GB520 19960308. PRIORITY: GB 1995-5538 19950318.

GI



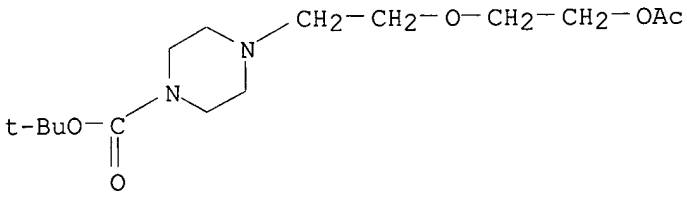
AB ArSO2AQ [Ar = (substituted) aryl, heterocyclyl; A = amino acid residue; Q = Q1, Q2; X = H, alkyl; Y = SO3H, PO(OR14)2, OH, SH, NR15R16, halo, (substituted) (CqH2q)Q3, etc.; Q3 = H, COR14, CO2R14, CONR15R16, SO3H, OR14, OCOR14, PO(OR14)2, NR15R16, SR14, halo; R14, R15, R16 = H, alkyl, cycloalkyl, aralkyl; R15R16N = 5-6 membered azacycloalkyl, oxazacycloalkyl; XY = O; Z = bond, O, N optionally substituted by X or Y; m, n = 2-4; m + n = 4-6, j, k = 0-2; j + k = 2-3; when A = Arg, then X, Y .noteq. alkyl; when Q = COR14, then q = 1-8], were prepd. Thus, (S)-arginine and 3-(1-methyl-1-phenylethyl)benzenesulfonyl chloride were stirred with Na2CO3 in H2O/dioxane to give 5-guanidino-2(S)-[3-(1-methyl-1-

phenylethyl)benzenesulfonylamino]pentanoic acid. The latter was converted to the acid chloride hydrochloride, which was condensed with pyrrolidin-2(R)-ylmethanol in DMF contg. Et3N to give N-[4-guanidino-1(S)-2(R)-hydroxymethylpyrrolidine-1-carbonylbutyl]-3-(1-methyl-1-phenylethyl)benzenesulfonamide. Tested title compds. inhibited human .alpha.-thrombin with Ki = 0.007-0.094 .mu.M.

IT **184042-78-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of arylsulfonylamino acid amide trypsin and thrombin inhibitors)

RN 184042-78-2 HCA

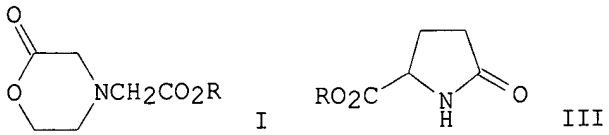
CN 1-Piperazinecarboxylic acid, 4-[2-[2-(acetyloxy)ethoxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L30 ANSWER 10 OF 27 HCA COPYRIGHT 2003 ACS on STN

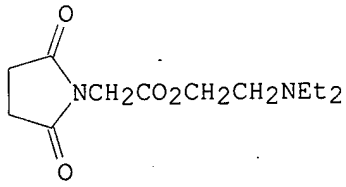
112:7866 Synthesis and inotropic activity of amino acid derivatives. Grinevich, A. I.; Kuznetsov, M. V.; Roshchupkina, O. V.; D'yachenko, V. Yu. (Kiev Med. Inst., Kiev, USSR). Farmatsevtichnii Zhurnal (Kiev) (1), 37-9 (Ukrainian) **1989**. CODEN: FRZKAP. ISSN: 0367-3057.

GI



I

III

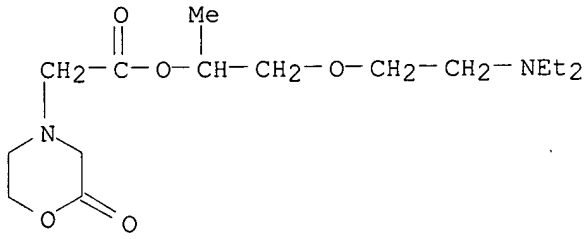


IV

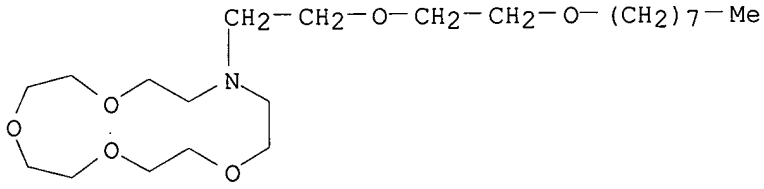
AB Cyclocondensation reaction of HO2CCH2CH2N(CH2CO2H)2 with ROH (R = Et2NCH2CH2OCH2CHMe, 1-morpholino-2-propyl) in refluxing xylene gave 53-64% (oxomorpholino)acetates I (same R). Analogous esterification of AcNHCHR1(CH2)nCO2H (R1 = H, n = 0, 1; R1 = Bu, n = 0) with ROH (R = same, Et2NCH2CH2) gave 5 corresponding AcNHCHR1(CH2)nCO2R (II) in 51-67% yield. Under these conditions, glutamic acid gave 41-54% oxopyrrolidinecarboxylates III (R = Et2NCH2CH2, Et2NCH2CHMe) and Me succinimidoacetate gave 32% imido ester IV. The inotropic activity of these compds. decreased in the order III > II > I > IV.

IT **124233-98-3P**

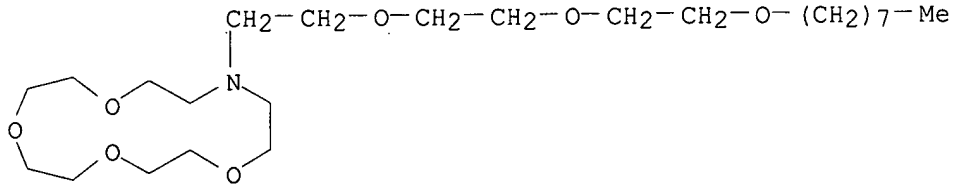
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and inotropic activity of)
RN 124233-98-3 HCA
CN 4-Morpholineacetic acid, 2-oxo-, 2-[2-(diethylamino)ethoxy]-1-methylethyl ester (9CI) (CA INDEX NAME)



L30 ANSWER 15 OF 27 HCA COPYRIGHT 2003 ACS on STN
99:11433 Proton driven active transport of alkali metal cations by using alkyl monoaza crown ether derivatives. Matsushima, Kenji; Kobayashi, Hirofumi; Nakatsuji, Yohji; Okahara, Mitsuo (Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, 577, Japan). Chemistry Letters (5), 701-4 (English) **1983**. CODEN: CMLTAG. ISSN: 0366-7022.
AB Octyl monoaza 18-crown-6 and the corresponding N lariat ethers are good carriers for the active transport of alkali metal cations. The transport ability correlates well with the complexing ability and the transport system makes use of the large difference in the complexing ability between the acidic and alk. phases.
IT **86170-84-5 86170-85-6 86170-87-8**
RL: DEV (Device component use); USES (Uses)
(membranes contg., for proton-driven active transport of alkali metal cations)
RN 86170-84-5 HCA
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-[2-(octyloxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)

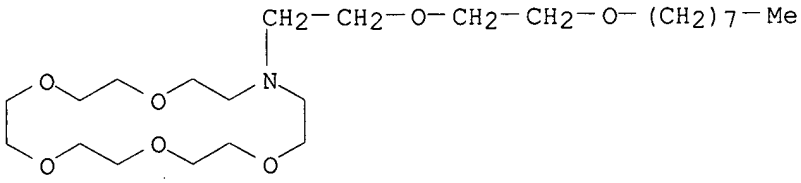


RN 86170-85-6 HCA
CN 1,4,7,10-Tetraoxa-13-azacyclopentadecane, 13-[2-[2-[2-(octyloxy)ethoxy]ethoxy]ethyl]- (9CI) (CA INDEX NAME)

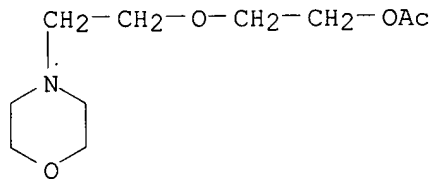


RN 86170-87-8 HCA

CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16-[2-[2-(octyloxy)ethoxy]ethyl]- (9CI) (CA INDEX NAME)



L30 ANSWER 20 OF 27 HCA COPYRIGHT 2003 ACS on STN
73:44672 Morpholinium compounds. Bogdal, Stanislaw (Polytech. Wroclaw, Wroclaw, Pol.). Roczniki Chemii, 44(1), 121-5 (Polish) **1970**. CODEN: ROCHAC. ISSN: 0035-7677.
GI For diagram(s), see printed CA Issue.
AB Pyrolysis of morpholinium salts (I) (X = OH, MeO, PhO, AcO) gave 2-morpholinoethyl vinyl ether (II), b15 94-5.degree., n20D 1.4684, d20 1.0018, 2-morpholinoethyl 2-phenoxyethyl ether (III), b5 182-3.degree., n20D 1.5192, d20 1.0853, and 2-morpholinoethyl 2-acetoxyethyl ether (IV), b8 146-7.degree., n20D 1.4605, d20 1.0810, depending on the anion X nucleophilicity. Thus, an aq. soln. of I (X = OH) was prepd. by shaking I (X = Cl) in 280 ml H2O with 20% excess of Ag2O and dilg. to 300 ml. When treated with 0.05 mole AcOH or PhOH 100 ml of the above soln. gave I (X = AcO) or I (X = PhO), resp. An alc. soln. of I (X = MeO) was prepd. from 0.05 mole I (X = Cl) and 0.05 mole MeONa in 75 ml MeOH. Evapn. of the solns. contg. I followed by heating at 150.degree. gave the following decompn. products (X, products, and % yield given): HO, II, 72; MeO, II, 77.2; PhO, II and III, 36.4 and 32.8; AcO, IV, 73.4.
IT **29293-94-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 29293-94-5 HCA
CN Ethanol, 2-[2-(4-morpholinyl)ethoxy]-, acetate (ester) (9CI) (CA INDEX NAME)



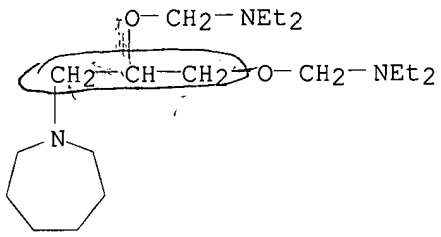
L30 ANSWER 25 OF 27 HCA COPYRIGHT 2003 ACS on STN
65:47598 Original Reference No. 65:8874d-g Ethers of glycols and their derivatives. CVI. Synthesis of alkoxymethyl ethers of 1-hexamethylenimino-2,3-propanediol. Mamedov, Sh.; Gadzhiev, F. R.; Khydyrov, D. N. (Inst. Petrochem. Processes, Baku). Zhurnal Obshchei Khimii, 2(4), 653-6 (Russian) **1966**. CODEN: ZOKHA4. ISSN: 0044-460X.
AB cf. CA 65, 8801a. Hexamethylenimine treated at 90-100.degree. with HOCH2CH(OH)CH2Cl and heated 12 hrs. longer gave 60% 1-hexamethyleniminopropane-2,3-diol (I), b3 127-9.degree., d20 1.0448, n20D 1.4940, which with MeOCH2Cl in the presence of powd. NaOH in C6H6 10 hrs. at 40.degree. gave 53% I bis(methoxymethyl ether), b3 130-2.degree., 1.0070, 1.4537; similarly were prepd. 50-65% yields of I diethers: bis(propoxymethyl), b3 156-8.degree., 0.9631, 1.4525; bis(butoxymethyl), b3 172-4.degree., 0.9522, 1.4542; bis(amyloxymethyl), b3 189-91.degree.,

0.9450, 1.4564; bis(isoamyloxymethyl), b3 181-3.degree., 0.9417, 1.4550. To 50 g. hexamethylenimine and 30 ml. H2O was added 18.5 g. epichlorohydrin at 10.degree. and after 12 hrs. at 90-100.degree. gave 78% 1,3-bis(hexamethylenimino)-2-propanol (II), b5 166-8.degree., 0.9718, 1.4970. This with ROCH2Cl and powd. NaOH, as above, gave 50-65% II ethers (CH2)6NCH2CH(OR)CH2N(CH2)6 (R given): methoxymethyl, b5 169-71.degree., 0.9774, 1.4884; propoxymethyl, b5 187-9.degree., 0.9610, 1.4820; butoxymethyl, b5, 200-2.degree., 0.9548, 1.4810; isobutoxymethyl, b5 194-6.degree., 0.9520, 1.4792; amyloxymethyl, b5 213-15.degree., 0.9508, 1.4806; isoamyloxymethyl, b5 208-10.degree., 0.9463, 1.4785. I and CH2:CHCN in the presence of MeONa in 7 hrs. at 50-60.degree. gave I bis(.beta.-cyanoethyl) ether, 53%, b1 166-8.degree., 1.0345, 1.4766; similarly prepd. was 65% II .beta.-cyanoethyl ether, b2 188-90.degree., 0.9840, 1.4906. I and paraformaldehyde with Et2NH in C6H6 gave in 25 hrs. heating 21% I bis(diethylaminomethyl) ether, b2 168-70.degree., 0.9400, 1.4750; similarly was prepd. 53% II diethylaminomethyl ether, b2 175-7.degree., 0.9412, 1.4860.

IT **6908-97-0**, Hexamethylenimine, 1-[2,3-bis[(diethylamino)methoxy]propyl]-
(prepn. of)

RN 6908-97-0 HCA

CN 1H-Azepine, 1-[2,3-bis[(diethylamino)methoxy]propyl]hexahydro- (8CI) (CA INDEX NAME)



L30 ANSWER 26 OF 27 HCA COPYRIGHT 2003 ACS on STN

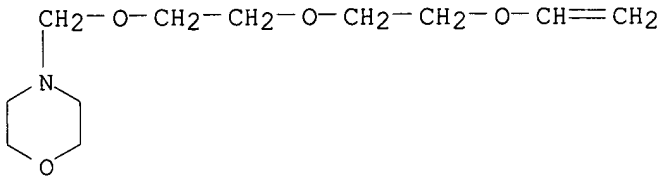
65:47158 Original Reference No. 65:8746b-d Vinyl ethers with terminal triple bond in the Mannich reaction. Atavin, A. S.; Trofimov, B. A.; Lavrov, V. I. (Inst. Org. Chem., Irkutsk). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (3), 543-4 (Russian) **1966**. CODEN: IASKA6. ISSN: 0002-3353.

AB Heating 6.7 ml. CH2:CHOCH2CH2OCH2CH2OCH2C.tplbond.CH with 1.8 g. paraformaldehyde and 5 ml. Et2NH in dioxane in the presence of 0.02 g. Cu2Cl2 2 hrs. at 90-100.degree. gave 69.6% CH2:CHOCH2CH2OCH2CH2OCH2C.tplbond.CNEt2, b1 120.degree., n20D 1.4692, d20 0.9714. Similarly were prepd. 53-70% CH2:CHOZOCH2C.tplbond.CNR'2 (Z and R' shown): CH2CH2, Et, b1 89.degree., 1.4672, 0.9379; (CH2CH2O)2CH2CH2, Et, b0.1 128.degree., 1.4690, 0.9841; (CH2)4, Et, b4 135.degree., 1.4667, 0.9230; (CH2)2CHMe, Et, b2 114.degree., 1.4631, 0.9213; (CH2CH2)2O, morpholino, b2 160.degree., 1.4891, 1.0668; (CH2CH2)2O, piperidino, b0.1 148.degree., 1.4881, 1.0145. Ir spectra were reported.

IT **10542-10-6**, Morpholine, 4-[[2-[2-(vinyloxy)ethoxy]ethoxy]methyl]-
(prepn. of)

RN 10542-10-6 HCA

CN Morpholine, 4-[[2-[2-(vinyloxy)ethoxy]ethoxy]methyl]- (7CI, 8CI) (CA INDEX NAME)



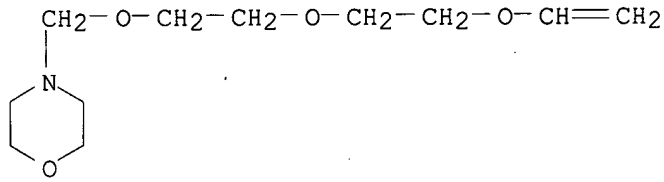
L30 ANSWER 27 OF 27 HCA COPYRIGHT 2003 ACS on STN
65:47157 Original Reference No. 65:8746a-b Dialkylaminomethoxy-substituted vinyl ethers. Shostakovslsii, M. F.; Atavin, A. S.; Lavrov, V. I.; Trofimov, B. A.; Bazanova, V. K. (Inst. Org. Chem., Irkutsk). Zhurnal Obshchei Khimii, 2(4), 597-600 (Russian) **1966**. CODEN: ZOKHA4. ISSN: 0044-460X.

AB Heating 13.2 g. HOCH2CH2OCH2CH2OCH: CH2 with 10.9 g. Et2NH and 3.6 g. paraformaldehyde in C6H6 with sepn. of resulting H2O (4 hrs.) gave 72.8% CH2:CH(OCH2CH2)2OCH2NEt2 (I), b2 94.degree., n20D 1.4428, d20 0.9363; similarly were prepd. 60% CH2:CHOCH2CH2OCH2NEt2, b1 45-50.degree., 1.4358, 0.8937; and 85% CH2:CH(OCH2CH2)3OCH2NEt2 b3 142.degree., 1.4480, 0.9645; 51.2% CH2:CH(OCH2CH2)2OCH2NC5H10, b1 108.degree., 1.4658, 0.9924; and 37% N-morpholino vinyl ether of diethylene glycol, b2 124.degree., 1.4670, 1.0534. I and EtSH in a sealed tube 8 days at room temp. gave 95% EtSCH2NEt2, b20 77.degree., 1.4685, 0.8884, and 91% CH2: CH(OCH2CH2)2H (II); I and MeOH in 5 days similarly gave 44.2% Et2NCH2OMe (b. 115.degree., 1.4058, 0.8165) and II. I and H2O in 4 hrs. gave 41.8% II. Ir spectra were reported.

IT **10542-10-6**, Morpholine, 4-[[2-[2-(vinyloxy)ethoxy]ethoxy]methyl]- (prepn. of)

RN 10542-10-6 HCA

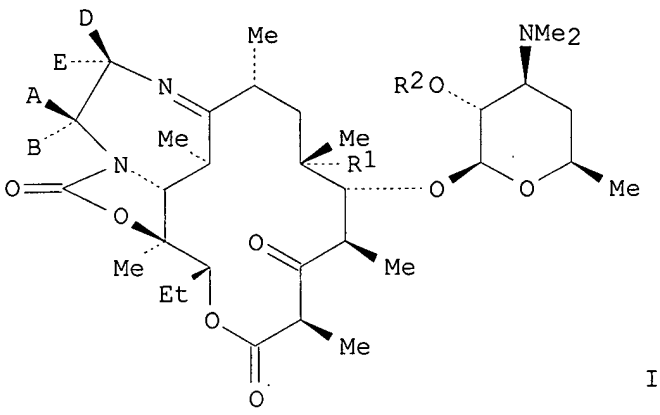
CN Morpholine, 4-[[2-[2-(vinyloxy)ethoxy]ethoxy]methyl]- (7CI, 8CI) (CA INDEX NAME)



=> d L30 2,4,6,8,11,13,17,19,21,23 cbib abs hitind hitstr

L30 ANSWER 2 OF 27 HCA COPYRIGHT 2003 ACS on STN
135:137676 Preparation of tricyclic erythromycins as bactericides. Or, Yat Sun; Phan, Ly Tam; Chu, Daniel T.; Spina, Kenneth P.; Hallas, Robert; Elliott, Richard L.; Tufano, Michael (Abbott Laboratories, USA). U.S. US 6274715 B1 20010814, 75 pp., Cont.-in-part of U.S. Ser. No. 555,246, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1997-779786 19970107. PRIORITY: US 1995-555246 19951108.

GI



I

AB Erythromycins I (A, B, D and E = independently H, alkyl, , aryl, heteroaryl, heterocycloalkyl, OH, alkoxy, halogen, amine; R1 = H, OH, alkyl, cycloalkyl, alkoxy, ester; R2 = H, OH protecting group) were prepd. as antibacterial agents. Thus, I (A = B = E = R1 = H, D = Bn, R1 = OMe) was prepd. and tested as antibacterial agent (MIC = 2-128).

IC ICM C07H017-08
ICS A61K031-70; A61P031-04

NCL 536007400

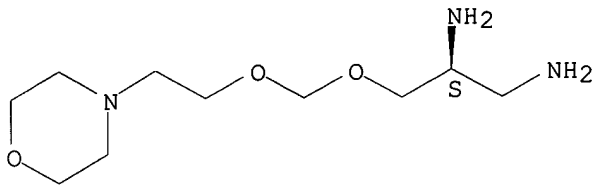
CC 33-7 (Carbohydrates)
Section cross-reference(s): 1, 63

IT 55-22-1, 4-Pyridinecarboxylic acid, reactions 62-23-7 74-11-3, 4-Chlorobenzoic acid 93-10-7, Quinoline-2-carboxylic acid 103-63-9, 2-Phenylethyl bromide 103-67-3, N-Benzylmethylamine 104-83-6, 4-Chlorobenzylchloride 106-93-4, 1,2-Dibromoethane 109-01-3, N-Methylpiperazine 486-74-8, Quinoline-4-carboxylic acid 585-71-7, 1-Phenylethyl bromide 589-10-6, 2-Phenoxyethyl bromide 637-59-2, 3-Phenylpropyl bromide 1068-90-2, Diethyl acetamidomalonate 1436-59-5, cis-1,2-Cyclohexanediamine 1477-50-5, 2-Indolecarboxylic acid 2124-55-2, 4-Indolecarboxylic acid 2130-96-3 2749-11-3, (S)-2-Amino-1-propanol 3182-95-4 3262-72-4 4065-92-3, 1,2-Cyclopentanediol 4358-64-9 5267-64-1 5339-26-4, 2-(4-Nitrophenyl)ethyl bromide 5341-95-7, meso-2,3-Butanediol 6482-24-2, 2-Methoxyethyl bromide 7252-83-7, 2,2-Dimethoxyethyl bromide 10316-79-7, 1-Amino-1-cyclopentanemethanol 10445-91-7, 4-Picolyl chloride 13139-17-8 14347-78-5 16136-58-6, 1-Methyl-2-indolecarboxylic acid 16793-89-8 16799-04-5 22323-82-6 23680-31-1 24347-58-8, (R,R)-2,3-Butanediol 24974-75-2 27038-09-1, (S)-Homophenylalaninol 29841-69-8 32233-43-5 35320-23-1, (R)-2-Amino-1-propanol 40535-45-3 52485-52-6 55533-25-0 78888-18-3 81103-11-9, Clarithromycin 85362-85-2 85803-43-6 135361-13-6 210554-89-5 210554-90-8 210554-95-3 210554-96-4 210554-97-5 210554-99-7 210555-00-3 210555-01-4 210555-06-9 210555-09-2 210555-10-5 210555-11-6 210555-12-7 210555-13-8 210555-14-9 210555-15-0 210555-16-1 210555-17-2 210555-18-3 **210555-19-4** 210555-20-7 210555-21-8 210555-22-9 210555-23-0 210555-24-1 210555-26-3 210555-27-4 210555-28-5 210555-29-6 210555-30-9 210555-31-0 210555-32-1 210555-33-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of tricyclic erythromycins as bactericides)

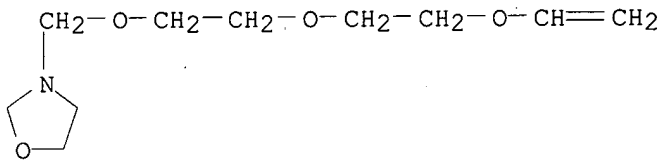
IT **210555-19-4**
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of tricyclic erythromycins as bactericides)
RN 210555-19-4 HCA
CN 1,2-Propanediamine, 3-[[2-(4-morpholinyl)ethoxy]methoxy]-, (2S)- (9CI) (CA INDEX NAME)

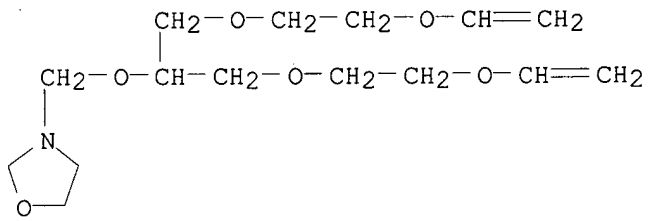
Absolute stereochemistry.



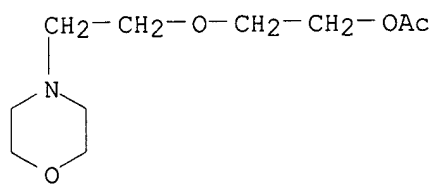
L30 ANSWER 4 OF 27 HCA COPYRIGHT 2003 ACS on STN
126:188778 Oxazolidines as efficient reagents for flotation of nonferrous and tungsten metal ores. Leonov, S.B.; Belkova, O. N.; Kukharev, B. F. (Irkutsk State Technical University, Irkutsk, Russia). Mineral Processing and Extractive Metallurgy Review, 16(3), 175-184 (English) **1996**. CODEN: MPERE8. ISSN: 0882-7508. Publisher: Gordon & Breach.
AB New representatives of oxazolidines have been prepd. by condensation of carbonyl compds. with aminoalcs. (compds. I-III), or by mutual condensation of formaldehyde with monoethanolamine and acyclic alcs. (compds. IV-IX) according to known methods. Oxazolidines I, II and IV-VII were tested as frothers in direct selective flotation of lead-zinc ores. Only oxazolidine I in the lead cycle is a worse frother than T-80. In the zinc cycle, the tested oxazolidines were better than oxal T-80 at consumption rates of 10 to 30 g/t. Compds. III, VIII and IX were tested as addnl. modifiers in collective flotation of copper-lead-zinc ores and xanthate flotation of primary scheelite ores. Compds. III and IX reduce WO3 losses both in the sulfide product and in the tailings of scheelite flotation. Oxazolidine III is a more efficient modifier than compd. IX. Compd. V was tested as a modifier in flotation of scheelite by sodium oleate at pH 9.3-9.6. Oxazolidine V improves the efficiency of sodium oleate in flotation of scheelite, which is due to changes in the proportions of the three forms of oxyhydrylic collector in the liq. phase of the pulp-ionic, mol., and micellar.
CC 54-1 (Extractive Metallurgy)
IT 90267-83-7 166896-08-8 166896-09-9 170877-60-8 187395-27-3 **187395-32-0 187395-33-1** 187395-34-2 187395-35-3
RL: NUU (Other use, unclassified); USES (Uses)
(flotation agent; oxazolidines as efficient reagents for flotation of Cu-Pb-Zn and scheelite ores)
IT **187395-32-0 187395-33-1**
RL: NUU (Other use, unclassified); USES (Uses)
(flotation agent; oxazolidines as efficient reagents for flotation of Cu-Pb-Zn and scheelite ores)
RN 187395-32-0 HCA
CN Oxazolidine, 3-[[2-[2-(ethenyloxy)ethoxy]ethoxy]methyl]- (9CI) (CA INDEX NAME)



RN 187395-33-1 HCA
CN Oxazolidine, 3-[[2-[2-(ethenyloxy)ethoxy]-1-[[2-(ethenyloxy)ethoxy]methyl]ethoxy]methyl]- (9CI) (CA INDEX NAME)



L30 ANSWER 6 OF 27 HCA COPYRIGHT 2003 ACS on STN
125:194974 Synthesis and nucleophilic substitution of esters of diethylene glycol chlorohydrin. Yakubov, A. V.; Zhanalieva, R. N.; Shakhidoyatov, Kh. M. (Inst. Khim. Rastit. Veshchestv, AN RUz, Uzbekistan). Uzbekskii Khimicheskii Zhurnal (4), 35-38 (Russian) **1995**. CODEN: UZKZAC. ISSN: 0042-1707. Publisher: Fan.
AB HOCH2CH2OCH2CH2Cl was esterified by carboxylic acids to give RCOOCH2CH2OCH2CH2Cl (I; R = H, Me, Et, Pr, ClCH2, Ph). Reaction of I with amines gave 2-[2-(acyloxy)ethoxy]ethylamines.
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 25, 27, 28
IT **29293-94-5P** 91343-57-6P 163231-46-7P 163231-47-8P
163231-48-9P 163231-49-0P 163231-50-3P 163231-51-4P 163231-52-5P
163231-53-6P 163231-54-7P 163231-55-8P 180619-47-0P 180619-48-1P
180619-49-2P 180619-50-5P 180619-51-6P 180619-52-7P 180619-53-8P
180619-54-9P 180619-55-0P 180619-56-1P 180619-57-2P 180619-58-3P
180619-59-4P 180619-60-7P 180619-61-8P 180619-62-9P 180619-65-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **29293-94-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 29293-94-5 HCA
CN Ethanol, 2-[2-(4-morpholinyl)ethoxy]-, acetate (ester) (9CI) (CA INDEX NAME)



L30 ANSWER 8 OF 27 HCA COPYRIGHT 2003 ACS on STN

122:313845 Reaction of .beta.-(.beta.'-acyloxyethoxy)ethyl chlorides with nucleophilic reagents. Zhanalieva, R. N.; Yakubov, A. V.; Shakhidoyatov, Kh. M.; Akhmedova, Sh. S. (Kaz. Gos. Natsional. Univ., Almaty, Kazakhstan). Izvestiya Natsional'noi Akademii Nauk Respubliki Kazakhstan, Seriya Khimicheskaya (3), 90-3 (Russian) **1994**. CODEN: INRKES. Publisher: Gylym.

AB Nucleophilic substitution reaction of RCO2CH2CH2OCH2CH2Cl (I; R = H, Me) with R''R'NH (e.g., anilines, dialkylamines, morpholine, piperidine) in presence of metal iodides (initial I/Cl exchange) afforded exclusively RCO2CH2CH2OCH2CH2NR'R'' in 39.3-83.1% yields. Yields were greater for R = H for a given amine, and also increased with amine basicity. Reaction of I (R = H) with NH4SCN afforded RCO2CH2CH2OCH2CH2SCN (68%).

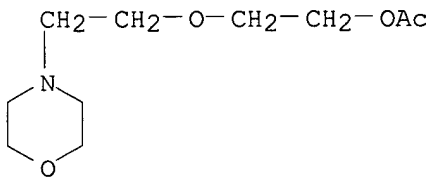
CC 21-2 (General Organic Chemistry)

IT **29293-94-5P** 91343-57-6P 163231-46-7P 163231-47-8P 163231-48-9P 163231-49-0P 163231-50-3P 163231-51-4P 163231-52-5P 163231-53-6P 163231-54-7P 163231-55-8P 163231-56-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(nucleophilic substitution reaction of .beta.-(.beta.'-acyloxyethoxy)ethyl chlorides with amines and thiocyanates)

IT **29293-94-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(nucleophilic substitution reaction of .beta.-(.beta.'-acyloxyethoxy)ethyl chlorides with amines and thiocyanates)

RN 29293-94-5 HCA

CN Ethanol, 2-[2-(4-morpholinyl)ethoxy]-, acetate (ester) (9CI) (CA INDEX NAME)



L30 ANSWER 11 OF 27 HCA COPYRIGHT 2003 ACS on STN

110:138522 Diaminoether compositions, their preparation and use for hydrogen sulfide removal from acidic gases. Stogryn, Eugene L.; Sartori, Guido (Exxon Research and Engineering Co., USA). U.S. US 4762934 A **19880809**, 10 pp. Cont.-in-part of U.S. Ser. No. 339,884, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1984-567569 19840103. PRIORITY: US 1982-339884 19820118.

AB Diaminoether compds. wherein one amino group thereof is a tertiary amine in N-heterocyclic form and the other amino group is a severely sterically hindered secondary amino group are useful in the selective removal of H2S from acidic gases and may be prepd. by a 3-step process. These compds. have a high selectivity for H2S in preference to CO2 which selectivity is maintained at high H2S and CO2 loading levels. Thus, 1-(pyrrolidinylethoxy)-2-(tert-butylaminoethoxy)ethane was prepd. and used to evaluate the selectivity for H2S in treating a gas mixt. contg. CO2 10, H2S 1, and N2 89 vol.%.

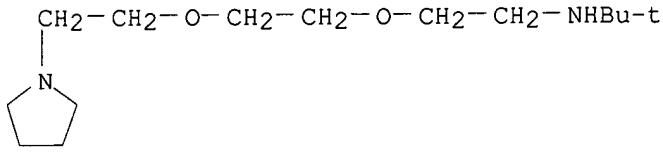
IC ICM C07D211-14
ICS C07D207-08; C07D223-04; C07D225-02

NCL 548569000

CC 51-11 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 27

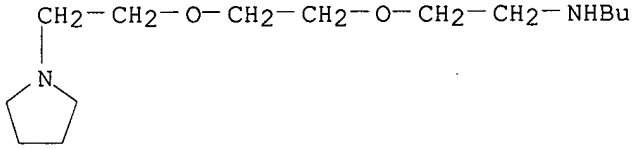
IT **114824-94-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and use of, for hydrogen sulfide removal from acidic gases)

IT **114824-94-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and use of, for hydrogen sulfide removal from acidic gases)
RN 114824-94-1 HCA
CN 2-Propanamine, 2-methyl-N-[2-[2-[2-(1-pyrrolidinyl)ethoxy]ethoxy]ethyl]- (9CI) (CA INDEX NAME)

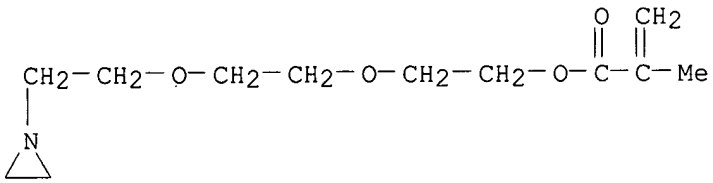


L30 ANSWER 13 OF 27 HCA COPYRIGHT 2003 ACS on STN
109:9218 Method for removal of sulfur compounds from CO2-containing gases.
Gazzi, Luigi; Rescalli, Carlo (SNAM Progetti S.p.A., Italy). Ger. Offen. DE 3717556 A1 **19871217**, 4 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 1987-3717556 19870525. PRIORITY: IT 1986-20757 19860611.
AB A method for selective removal of H2S and other S-contg. compds., e.g., COS, CS2, and mercaptans from CO2-contg. gases (esp. natural gas and synthesis gas comprises applying a wash soln. contg. tertiary amines and/or sterically hindered primary and/or secondary amines in the form of diaminoethers or aminoalcs.) in water and org. solvent (if desired), regenerating the spent wash liq., mixing the regenerated wash liq. with the gases leaving the absorber, and recycling the wash liq. to the top of the absorber after cooling of the resulting mixt. Thus, a CO2-contg. gas (contg. H2S 1.6, CO2 12.5, CH4 85.864, COS 0.017, and CH3SH 0.019 vol.%) was treated in accordance with the invention by using a 50% aq. soln. of methyldiethanolamine; the vol. of the circulating wash soln. was reduced.
IC ICM B01D053-14
ICS C10K001-16; B01D047-10
CC 51-5 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 48
IT 96-80-0 100-37-8 105-59-9 108-01-0, Dimethylethanolamine 139-87-7, Ethyldiethanolamine 4620-70-6, tert-Butylaminoethanol 7005-47-2, N,N-Dimethyl-2-amino-2-methylpropan-1-ol 10342-97-9, Methyldiisopropylamine 15521-18-3, N,N-Dimethyl-2-amino-propan-1-ol 18366-39-7, 2-tert-Butylamino-1-propanol 18366-44-4 20919-81-7, Propyldiisopropanolamine 24403-02-9, 2-Isopropylamino-1-propanol 63246-63-9 72562-31-3, 1,2-Bis(pyrrolidinylethoxy)ethane 73732-79-3, (3-tert-Butylamino)-n-butanol 76331-19-6, 1,2-Bis(pyperidinylethoxy)ethane 87787-68-6 87787-69-7, 2-(2-tert-Butylamino)propoxyethanol 87787-71-1, tert-Amylaminoethoxyethanol 87787-72-2, N-Methyl-N-tert-butylaminoethoxyethanol 87787-73-3, 2-(N-Isopropyl-N-methylamino)propoxyethanol 87787-74-4, 3-Aza-2,2,3-trimethyl-1,6-hexanediol 87787-76-6 99337-13-0, 1,2-Bis(tert-butylaminoethoxy)ethane 100396-39-2, Bis(N-pyrrolidinylethyl)ether 114824-92-9, N,N-Dimethyl-2-amino-2-methylbutan-1-ol 114824-93-0, 2-Methyl-2-(methyl-.beta.-hydroxyethylamino)-1-propanol **114824-94-1**, 1-(Pyrrolidinylethoxy)-2-(tert-butylaminoethoxy)ethane 114824-95-2, (1-Methyl-1-ethylpropylamino)ethoxyethanol 114824-96-3, Bis(tert-butylaminoethyl)ether 114824-97-4, Bis(2-isopropylaminopropyl)ether 114824-98-5, 1,2-Bis-(3-pyrrolidinyl-n-propoxy)ethane
RL: USES (Uses)
(wash solns. contg., for desulfurization of carbon dioxide-contg. gases)

IT **114824-94-1**, 1-(Pyrrolidinylethoxy)-2-(tert-butylaminoethoxy)ethane
RL: USES (Uses)
(wash solns. contg., for desulfurization of carbon dioxide-contg. gases)
RN 114824-94-1 HCA
CN 2-Propanamine, 2-methyl-N-[2-[2-[2-(1-pyrrolidinyl)ethoxy]ethoxy]ethyl]- (9CI) (CA INDEX NAME)

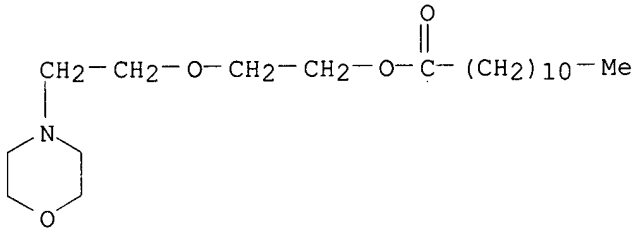


L30 ANSWER 17 OF 27 HCA COPYRIGHT 2003 ACS on STN
87:23484 Silanes having an amine functional group thereon. Mitchell, Tyrone D. (General Electric Co., USA). Can. CA 995227 **19760817**, 23 pp. (English). CODEN: CAXXA4. APPLICATION: CA 1972-149425 19720815.
AB (MeO)3Si(CH2)3ZH [Z = NH(I), S, OCH2CHMeCH2NH] and (EtO)3Si(CH2)3OH reacted with 2-aziridinoethyl methacrylate at 100.degree. to give (MeO)3Si(CH2)3ZCH2CHMeCO2CH2CH2R (R = aziridino) and (EtO)3Si(CH2)3OCH2CHMeCO2CH2CH2R, resp. I reacted analogously with CH2:CMeCO(OCH2CH2)3R (R = aziridino).
CC 29-6 (Organometallic and Organometalloidal Compounds)
IT **63120-82-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(addn. reaction of, with (aminopropyl)trimethoxysilane)
IT **63120-82-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(addn. reaction of, with (aminopropyl)trimethoxysilane)
RN 63120-82-1 HCA
CN 2-Propenoic acid, 2-methyl-, 2-[2-[2-(1-aziridinyl)ethoxy]ethoxy]ethyl ester (9CI) (CA INDEX NAME)

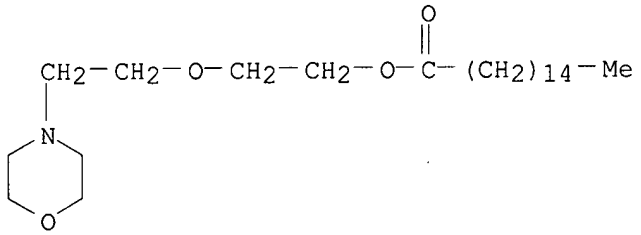


L30 ANSWER 19 OF 27 HCA COPYRIGHT 2003 ACS on STN
78:124600 N-[3-(2'-Acyloxyethoxy)-ethyl]-morpholines. Ozaki, Shoichiro; Takahashi, Toru (Mitsui Toatsu Chemicals Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 48013373 **19730220** Showa, 4 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1971-45687 19710625.
GI For diagram(s), see printed CA Issue.
AB The title compds. (I), useful as surfactants, plasticizers, and catalysts, were prepd. by acylating N-[2-(2-hydroxyethoxy)ethyl]morpholine (II). E.g. 8.67 g II was dropped into 10.58 g hot lauroyl chloride to give 19.3 g I (acyl = lauroyl). Similarly prepd. were 2 more I where acyl = palmitoyl and caproyl.
NCL 16E451.1
CC 28-14 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 36, 46

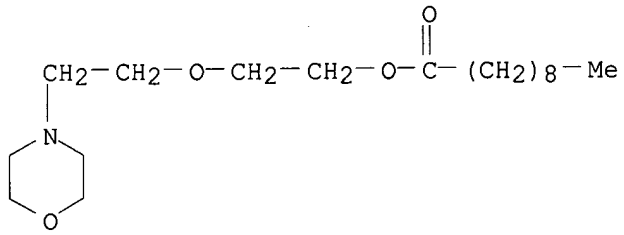
IT **41554-53-4P 41554-54-5P 41583-02-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **41554-53-4P 41554-54-5P 41583-02-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 41554-53-4 HCA
CN Dodecanoic acid, 2-[2-(4-morpholinyl)ethoxy]ethyl ester (9CI) (CA INDEX NAME)



RN 41554-54-5 HCA
CN Hexadecanoic acid, 2-[2-(4-morpholinyl)ethoxy]ethyl ester (9CI) (CA INDEX NAME)



RN 41583-02-2 HCA
CN Decanoic acid, 2-[2-(4-morpholinyl)ethoxy]ethyl ester (9CI) (CA INDEX NAME)



L30 ANSWER 21 OF 27 HCA COPYRIGHT 2003 ACS on STN
71:12449 Vinyl ethers containing functional groups and heteroatoms. Lavrov, V. I.; Atavin, A. S.; Trofimov, B. A.; Nikitin, V. M.; Vyalykh, E. P. (USSR). Khimiya Atsetilena, Doklady Vsesoyuznoi Nauchnoi Konferentsii po Khimii Atsetilena i Ego Proizvodnykh 278-81 From: Ref. Zh., Khim. 1968, Abstr. No. 20Zh152 (Russian) **1968**. CODEN: 20WJAZ.
AB By cyanoethylation, aminomethylation, and by interaction of CH2:CH(CH2CH2)nOH with ClSiMe3 and ClSnEt3 in strong basic medium, the following vinyl ethers were synthesized contg. functional groups and heteroatoms (compd., b.p., n20D, and d20 given): CH2:CH(OCH2CH2)2CN (I), b4 96.degree., 1.4468, 1.0077; CH2:CHO(CH2)3OCH2CH2CN (II), b1 89.degree.,

1.4450, 0.9801; CH2:-CHO(CH2)4OCH2CH2CN (III), b2 103.degree., 1.4476, 0.9698; CH2:-CHOCH2CH2CHMeOCH2CH2CN (IV), b1 88.degree., 1.4429, 0.9664; CH2:CH(OCH2)3CN (V), b4 125.5.degree., 1.4532, 1.0368; CH2:CH(OCH2CH2)4CN (VI), b2 136.degree., 1.4568, 1.0527; CH2:CHOCH2CH2OCH2NEt2 (VII), b1 40-50.degree., 1.4358, 0.8937; CH2:CH(OCH2CH2)2OCH2NEt2 (VIII), b2 94.degree., 1.4428, 0.9363; CH2:CH(OCH2CH2)3OCH2NEt2 (IX), b3 142.degree., 1.4480, 0.9645; RCH2O(CH2CH2O)2CH:CH2 (R = piperidino) (X), b1 108.degree., 1.4658, 0.9924; RCH2O(CH2CH2O)2CH:CH2 (R = morpholino) (XI), b2 124.degree., 1.4670, 1.0534; CH2:CHOCH2CH2OSiMe3 (XII); b715 147.degree., 1.4139, 0.8640; CH2:CH(OCH2CH2)2OSiMe3 (XIII), b11 85.degree., 1.4260, 0.9175; CH2:CH(OCH2CH2)3OSiMe3 (XIV), b2 80.degree., 1.4343, 0.9475; CH2:CHOCH2CH2OSnEt3 (XVI), b3 99.95.degree., 1.4810, 1.2565; CH2:CH(OCH2CH2)2OSnEt3 (XVI), b2 119.0-9.5.degree., 1.4809, 1.2456; CH2:CH(OCH2CH2)3SnEt3 (XVII), b1 136.0-6.5.degree., 1.4780, 1.2145. Redn. of I-VI with LiAlH4 instead of the formation of the expected NH2-contg. vinyl esters, C-O bonds in the NCCH2CH2O group split; redn. of I-VI with Na in alc. occurred with the transfer of the NCCH2CH2O group and gave (after hydrolysis of the formed ethers) HOCH2CH2OCH2CH2CN, b3 120.degree., n20D 1.4442, d20 1.0823, and HOCH2CH2(OCH2CH2)2CN, b1 118.degree., n20D 1.4520, d20 1.0943. Interaction of I with alc. gave MeCH(OEt)OCH2CH2OCH2CH2CN, b1 100.degree., n20D 1.4340, d20 1.0049. Capacity of the CH2:CHO group in VII-XI for electrophilic addn. was suppressed: on their interaction with ROH and RSH instead of the expected addn. a splitting of C-O-bonds occurred in the R2NCH2O group with the formation of monovinyl glycol ethers and MeOCH2NEt2, b730 115.degree., n20D 1.4058, d20 0.8165, and EtSCH2NEt2, b20 77.degree., n20D 1.4685, d20 0.8884, resp. Reaction of VII-XI with water led to the corresponding monovinyl esters. XII-XIV ethers in the absence of added acids were combined with EtSH exclusively by the radical mechanism with the formation of the corresponding EtSCH2CH2(OCH2CH2)nOSiMe3 (XVIII) (n, b.p., n20D, and d20 given): 1, b481.degree., 1.4505, 0.9380; 2, b3.1 112.degree., 1.4525, 0.9615; 3, b3 142.degree., 1.4569, 0.9872. Hydrolysis of XVIII (n = 1) led to EtSCH2CH2OCH2CH2OH, b3 88.degree., n20D 1.4820, d20 1.0433, the structure of which was confirmed by the addn. of EtSH to CH2:CHOCH2CH2OH. XV-XVIII did not polymerize under the effect of FeCl3, ZnCl2, and (PhCOO)2 and did not add ROH in the presence of acid catalysts.

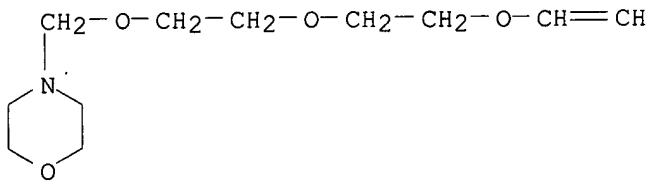
CC 23 (Aliphatic Compounds)

IT 1608-80-6P 1608-81-7P 1743-11-9P 2097-64-5P 2097-65-6P
2288-03-1P 3492-69-1P 3492-79-3P 3944-79-4P 3944-81-8P
4885-30-7P 4885-31-8P 4885-32-9P 4885-33-0P 4885-34-1P
4885-35-2P 4885-36-3P 5888-29-9P 7109-24-2P 10143-54-1P
10542-09-3P **10542-10-6P** 24298-23-5P 24298-24-6P
24298-26-8P 24298-27-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **10542-10-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 10542-10-6 HCA

CN Morpholine, 4-[[2-[2-(vinyloxy)ethoxy]ethoxy]methyl]- (7CI, 8CI) (CA INDEX NAME)



L30 ANSWER 23 OF 27 HCA COPYRIGHT 2003 ACS on STN
68:12380 Glycerol diether hydroxides with a propargylic substituent. Gautier, Jean A.; Miocque, Marcel; Fauran, Claude; Douzon, Colette (Fac. Pharm, Paris, Paris, Fr.). Bulletin de la Societe Chimique de France (9), 3190-5 (French) **1967**. CODEN: BSCFAS. ISSN: 0037-8968.

AB The synthesis of 1,3-disym. diether hydroxides, ROCH2CH(OH)CH2OCH2C.tplbond.CH (I) from glycerol, propargyl alc., and an aliphatic or aromatic alc. is described. Thus, 1 mole epichlorohydrin is treated with 3 moles HC.tplbond.cCH2OH in the presence of BF3.Et2O at 40-50.degree. to give ClCH2CH(OH)CH2OCH2C.tplbond.CH (II), b0.2 82.degree.. II was transformed with a slight excess of NaOH at 0-5.degree. to 1-propargyloxy-2,3-epoxypropane (III), b7 58.degree., and III converted to I by 1 of 3 methods. For satd. aliphatic, ethylenic, and chlorohydrin alcs., 0.5 mole III is treated with 1.5 moles of the alc. in the presence of BF3. Et2O; when the alc. is aromatic, 1 mole III is treated with 1 mole of the alc. in the presence of Na at 20-60.degree.; or when the alc. is a morpholinoalkanol, 1 mole 1-propargyloxy-3-(3-chloro-1-alkyloxy)-2-propanol is reacted with 2.5 moles morpholine. I are further transformed into their carbamate derivs. ROCH2CH(O2CNH2)CH2OCH2C.tplbond.CH (IV), by the successive action of COCl2 in the presence of a tertiary amine, e.g. Et3N or PhNEt2. The compds. prepd. are characterized by their elemental anal., acetylenic H detn., ir spectra, and phys. consts. Compds. prepd. are tabulated. [TABLE OMITTED] Also prepd. were those compds. in the 2nd table. Also reported was IV (R = PhCHMe), b0.01 185-9.degree., n20D 1.5170. [TABLE OMITTED]

CC 23 (Aliphatic Compounds)

IT 14669-14-8P 14669-15-9P 14669-16-0P 14669-17-1P 14669-18-2P
14669-19-3P 14714-99-9P 14715-00-5P 16169-00-9P 16169-02-1P
16169-03-2P 16169-05-4P 16169-06-5P 16169-07-6P 16169-08-7P
16169-09-8P 16169-10-1P 16169-11-2P 16169-19-0P 16169-20-3P
16169-21-4P 16169-22-5P 16169-23-6P 16169-24-7P 16221-28-6P
16221-29-7P 16221-30-0P 16221-31-1P 16221-32-2P 16221-33-3P
16221-34-4P 16221-35-5P 16221-36-6P 16221-37-7P 16221-38-8P
16221-39-9P 16221-40-2P 16221-41-3P 16221-42-4P 16221-43-5P
16221-44-6P 16221-45-7P 16221-46-8P 16221-47-9P 16221-48-0P
16221-49-1P 16221-50-4P 16221-52-6P 16221-54-8P 16221-55-9P
16221-56-0P 16221-58-2P 16221-59-3P 16221-60-6P 16221-61-7P
16221-62-8P 16221-63-9P 16221-65-1P **16221-66-2P**
16221-67-3P 16221-68-4P 16221-69-5P 16222-49-4P 16222-50-7P
16222-52-9P 16222-53-0P 16222-54-1P 16222-55-2P 16222-56-3P
16271-95-7P 16271-96-8P 16271-97-9P 16271-98-0P 16272-01-8P
16991-89-2P 18180-29-5P 18180-30-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **16221-66-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 16221-66-2 HCA

CN 2-Propanol, 1-(2-morpholinoethoxy)-3-(2-propynyloxy)-, carbamate (ester) (8CI) (CA INDEX NAME)